Minimal Efficiency of Experimental Designs under the Class of Orthogonally Invariant Criteria

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Part I

INTRODUCTION

Chapter 1
FUNDAMENTALS, TERMINOLOGY, NOTATION

In this chapter, we will give a brief introduction to the theory of optimal design of uncorrelated linear regression experiments with focus on the terminology and notation used in the rest of the thesis. For a more detailed explanation of foundations of the theory of optimal experimental design, we refer the reader to the monographs [17] and [19].

1.1 Experimental designs, information matrices and the Elfving set

Consider the linear regression model on a compact experimental domain $\mathfrak{X} \subseteq \mathfrak{R}^s$. For each design point $x \in \mathfrak{X}$, we can observe a random variable

$$y = f^T(x)\beta + \varepsilon$$

where $f : \mathfrak{X} \to \mathfrak{R}^m$ is a known vector of regression functions, $\beta \in \mathfrak{R}^m$ is an unknown vector of parameters, and ε is an unobservable random error. We suppose that the components of f are continuous and linearly independent real functions. For different observations, the errors are assumed to be uncorrelated, with zero mean and the same variance, which is assumed to be 1 without loss of generality. We will denote this model by $(f, \mathfrak{X})$ and say that $(f, \mathfrak{X})$ is m-dimensional.

As is usual in the asymptotic theory, by an experimental design we understand a probability measure ξ finitely supported on $\mathfrak{X}$. For an experimenter, the value $\xi(x)$ determines the relative proportion of the measurements that should be taken in $x \in \mathfrak{X}$. The set of all designs on $\mathfrak{X}$ will be denoted by $\Xi_{\mathfrak{X}}$. Evidently, the set $\Xi_{\mathfrak{X}}$ is convex.

The performance of a design $\xi \in \Xi_{\mathfrak{X}}$ is based on the information matrix associated with ξ, which is a positive semidefinite matrix defined by the formula

$$\mathbf{M}_{f,\mathfrak{X}}(\xi) = \sum_{x \in \mathfrak{X};\, \xi(x) > 0} \xi(x)\, f(x) f^T(x)$$

If we perform n experiments in accord with a design ξ, and if $\mathbf{M}_{f,\mathfrak{X}}(\xi)$ is regular, then $n\mathbf{M}_{f,\mathfrak{X}}(\xi)$ is equal to the inverse of the covariance matrix of the least squares estimate of β. Moreover, if the observations are normally distributed, then $n\mathbf{M}_{f,\mathfrak{X}}(\xi)$ is the Fisher information matrix for the parameter β. Hence, roughly speaking, $\mathbf{M}_{f,\mathfrak{X}}(\xi)$ is the average Fisher information matrix for the unknown parameter that can be attributed to a single observation executed in accord with the experimental plan ξ.

The assumptions given above imply that the set $\mathcal{M}_{f,\mathfrak{X}} = \{\mathbf{M}_{f,\mathfrak{X}}(\xi) : \xi \in \Xi_{\mathfrak{X}}\}$ of all information matrices is convex, compact and contains a regular matrix (see e.g. [17], p. 60).

The Elfving set of the model $(f, \mathfrak{X})$ is a compact subset of $\mathfrak{R}^m$ defined by

$$\mathfrak{E}_{f,\mathfrak{X}} = \operatorname{conv}\{-f(\mathfrak{X}) \cup f(\mathfrak{X})\}$$

Let $\mathcal{P}_{m,k}$ be the set of all orthogonal projectors which project $\mathfrak{R}^m$ onto a k-dimensional linear subspace of $\mathfrak{R}^k$, $k \in \{1, ..., m\}$. For the purpose of this work, we introduce the k-radius of the Elfving set:

$$r_k(\mathfrak{E}_{f,\mathfrak{X}}) = (1/2) \times \min\nolimits_{\mathbf{P} \in \mathcal{P}_{m,k}} \operatorname{diam}(\mathbf{P}\mathfrak{E}_{f,\mathfrak{X}})$$

The k-radius of $\mathfrak{E}_{f,\mathfrak{X}}$ can be geometrically interpreted as the minimal possible radius of the k-dimensional base of a "cylinder" circumscribed to $\mathfrak{E}_{f,\mathfrak{X}}$. It is simple to show that $r_1(\mathfrak{E}_{f,\mathfrak{X}})$ is the radius of the sphere inscribed to $\mathfrak{E}_{f,\mathfrak{X}}$ and $r_m(\mathfrak{E}_{f,\mathfrak{X}})$ is the radius of the sphere circumscribed to $\mathfrak{E}_{f,\mathfrak{X}}$.

1.2 Optimality and efficiency of designs

An optimality criterion is a real valued matrix function Φ which measures the largeness of an information matrix, i.e. the quality of the corresponding design. We say that a design ξ^* is optimal for the model $(f, \mathfrak{X})$ with respect to an optimality criterion Φ or, equivalently, that ξ^* is Φ-optimal for $(f, \mathfrak{X})$ iff

$$\Phi(\mathbf{M}_{f,\mathfrak{X}}(\xi^*)) = \sup\nolimits_{\zeta \in \Xi_{\mathfrak{X}}} \Phi(\mathbf{M}_{f,\mathfrak{X}}(\zeta))$$

In this case, $\mathbf{M}_{f,\mathfrak{X}}(\xi^*)$ is called an optimal information matrix for the model $(f, \mathfrak{X})$ with respect to the criterion Φ, or Φ-optimal for $(f, \mathfrak{X})$. The value $\Phi(\mathbf{M}_{f,\mathfrak{X}}(\xi^*))$ is then called the Φ-optimal value of $(f, \mathfrak{X})$.

For a nonnegative criterion Φ, which is not identically 0 on $\mathcal{M}_{f,\mathfrak{X}}$, we define the Φ-efficiency of a design $\xi \in \Xi_{\mathfrak{X}}$ in the form

$$\operatorname{eff}_{f,\mathfrak{X}}(\xi|\Phi) = \frac{\Phi(\mathbf{M}_{f,\mathfrak{X}}(\xi))}{\sup_{\zeta \in \Xi_{\mathfrak{X}}} \Phi(\mathbf{M}_{f,\mathfrak{X}}(\zeta))}$$

The efficiency $\operatorname{eff}_{f,\mathfrak{X}}(\xi|\Phi)$ can be interpreted as the extent to which the design ξ exhausts the maximum amount of information about the parameter.

We remark that if the model we analyze is obvious from the context, or if the results that are being presented pertain to all models, we suppress the symbols f and $\mathfrak{X}$ in the above-defined notation. In this case $\Xi_{\mathfrak{X}}$, $\mathbf{M}_{f,\mathfrak{X}}$, $\mathcal{M}_{f,\mathfrak{X}}$, $\mathfrak{E}_{f,\mathfrak{X}}$ and $\operatorname{eff}_{f,\mathfrak{X}}$ become Ξ, $\mathbf{M}$, $\mathcal{M}$, $\mathfrak{E}$, and eff.

Let the symbols $\mathcal{S}^m$, $\mathcal{S}^m_+$, and $\mathcal{S}^m_{++}$ denote the sets of all symmetric, positively semidefinite, and positively definite matrices of type $m \times m$. On $\mathcal{S}^m$ we use the

Loewner partial ordering $\leq$, which is defined as $\mathbf{A} \leq \mathbf{B}$ iff $\mathbf{B} - \mathbf{A} \in \mathcal{S}_+^m$. Moreover, for $\mathbf{A} \in \mathcal{S}^m$ we define $\lambda(\mathbf{A}) = (\lambda_1(\mathbf{A}), \ldots, \lambda_m(\mathbf{A}))^T$ - the vector of all (not necessarily distinct) eigenvalues of $\mathbf{A}$ in nondecreasing order:

$$\lambda_1(\mathbf{A}) \leq \lambda_2(\mathbf{A}) \leq ... \leq \lambda_m(\mathbf{A})$$

Clearly, $\lambda(\mathbf{A})$ has nonnegative (positive) components for all $\mathbf{A} \in \mathcal{S}_+^m$ (resp. $\mathbf{A} \in \mathcal{S}_{++}^m$).

1.3 Orthogonally invariant criteria

An orthogonally invariant criterion is any matrix function $\Phi : \mathcal{S}_+^m \to [0, \infty)$ which is not identically zero, and which satisfies the following general properties:

(I) *isotonicity:*
$\mathbf{C} \leq \mathbf{D} \Rightarrow \Phi(\mathbf{C}) \leq \Phi(\mathbf{D})$ for all $\mathbf{C}, \mathbf{D} \in \mathcal{S}_+^m$

(C) *concavity:*
$\Phi(\alpha\mathbf{C} + (1-\alpha)\mathbf{D}) \geq \alpha\Phi(\mathbf{C}) + (1-\alpha)\Phi(\mathbf{D})$ for all $\mathbf{C}, \mathbf{D} \in \mathcal{S}_+^m$ and $\alpha \in [0, 1]$

(S) *upper semicontinuity:*
The level sets $\left\{\mathbf{C} \in \mathcal{S}_+^m : \Phi(\mathbf{C}) \geq c\right\}$ are closed for all $c \in \Re$

(H) *positive homogeneity:*
$\Phi(\alpha\mathbf{C}) = \alpha\Phi(\mathbf{C})$ for all $\mathbf{C} \in \mathcal{S}_+^m$ and $\alpha \geq 0$

(O) *orthogonal invariance:*
$\Phi\left(\mathbf{U}\mathbf{C}\mathbf{U}^T\right) = \Phi(\mathbf{C})$ for all $\mathbf{C} \in \mathcal{S}_+^m$ and orthogonal $m \times m$ matrices $\mathbf{U}$

A criterion satisfying (I),(C),(S),(H) is sometimes called an information function (see [19], Chapter 5 for a thorough argumentation in favor of these properties). If Φ is an information function, then the sets of all Φ-optimal designs and all Φ-optimal information matrices are nonempty and convex. Moreover, the Φ-optimal value is positive (cf. Lemma 5.16. in [19]).

The property (O) will be analysed in Section 3.1, where we show why is the property of orthogonal invariance natural for the criteria which simultaneously measure quality of estimation of all components of β. We denote the class of all orthogonally invariant criteria by the symbol $\mathbb{O}$.

The most important examples of orthogonally invariant criteria are the Kiefer's criteria of Φ_p-optimality for $p \in [-\infty, 1]$. (We use the parametrization as defined in [19] p. 139,140, which differs from the classical "convex" definition; cf. [17] p. 94.)

$$\Phi_p(\mathbf{C}) = \begin{cases} \lambda_1(\mathbf{C}) & \text{if } p = -\infty \\ \left(\frac{1}{m}\sum_{i=1}^m \lambda_i^p(\mathbf{C})\right)^{1/p} & \text{if } p \in (-\infty, 0) \text{ and } \mathbf{C} \in \mathcal{S}_{++}^m \text{ or if } p \in (0, 1] \\ \left(\prod_{i=1}^m \lambda_i(\mathbf{C})\right)^{1/m} & \text{if } p = 0 \\ 0 & \text{if } p \in (-\infty, 0) \text{ and } \mathbf{C} \in \mathcal{S}_+^m \backslash \mathcal{S}_{++}^m \end{cases}$$

Some extensively studied special cases are exhibited in the following table.

Name	Criterion	For $\mathbf{C} \in \mathcal{S}_{++}^m$	For $\mathbf{C} \in \mathcal{S}_{+}^m \backslash \mathcal{S}_{++}^m$
E-optimality	$\Phi_{-\infty}$	$\lambda_1(\mathbf{C})$	0
A-optimality	Φ_{-1}	$m\left(\mathrm{tr}(\mathbf{C}^{-1})\right)^{-1}$	0
D-optimality	Φ_0	$\left(\det(\mathbf{C})\right)^{1/m}$	0
T-optimality	Φ_1	$m^{-1}\,\mathrm{tr}(\mathbf{C})$	$m^{-1}\,\mathrm{tr}(\mathbf{C})$

The class $\mathbb{O}$ also contains the criteria of Ch_k-optimality (characteristic polynomial criteria; see [24], or [25]) for all $k = 1, ..., m$ defined in their homogeneous and concave version:

$$\Phi_{Ch_k}(\mathbf{C}) = \left(\binom{m}{k}^{-1} \sum_{1 \le i_1 < ... < i_k \le m} \lambda_{i_1}^{-1}(\mathbf{C}) ... \lambda_{i_k}^{-1}(\mathbf{C})\right)^{-1/k} \quad \text{for } \mathbf{C} \in \mathcal{S}_{++}^m$$

We define $\Phi_{Ch_k}(\mathbf{C}) = 0$ for $\mathbf{C} \in \mathcal{S}_{+}^m \backslash\ \mathcal{S}_{++}^m$. Notice that the criterion Φ_{Ch_1} is identical to the criterion of A-optimality and Φ_{Ch_m} is the criterion of D-optimality, but other characteristic polynomial criteria do not correspond to any of the criteria of Φ_p-optimality.

In this work, we introduce a new class of criteria, which we call criteria of E_k-optimality. For $k \in \{1, ..., m\}$ we define the criterion of E_k-optimality by

$$\Phi_{E_k}(\mathbf{C}) = \sum_{i=1}^{k} \lambda_i(\mathbf{C}) \text{ for all } \mathbf{C} \in \mathcal{S}_{+}^m$$

Clearly, the criterion of E_1-optimality is equivalent to the criterion of E-optimality and the criterion of E_m-optimality corresponds to a constant multiple of the criterion of T-optimality. In Section 3.2 we will show that any criterion Φ_{E_k} belongs to $\mathbb{O}$.

Apart from the criteria defined above, there is a richness of other orthogonally invariant criteria, since any convex combination, or a minimum of a finite set of criteria from $\mathbb{O}$ is again an orthogonally invariant criterion (cmp. [19], p.124-125).

For the $\Phi_{-\infty}$-, Φ_{-1}-, Φ_0-, Φ_1-, Φ_{E_k}-optimal designs (optimal matrices, optimal values, efficiencies) we will also use the concise terminology E-, A-, D-, T-, and E_k-optimal designs (optimal matrices, optimal values, efficiencies).

Chapter 2
FORMULATION OF THE AIM AND DESCRIPTION OF THE MAIN RESULTS OF THE THESIS

2.1 The aim of the thesis

Much of the effort in optimal design of experiments is aimed at solving the following type of problems: For the model $(f, \mathfrak{X})$ in consideration, find the design of best performance measured by a *fixed* criterion of optimality. Often, though, it is very difficult to give a persuasive justification for the choice of a single criterion, because there is a large number of different criteria, *all* of which measure useful aspects of designs.

The same problem was formulated by Galil and Kiefer in the following citation introducing the article [6]:

"A first step away from the traditional choice of a design to satisfy some principle of intuition or symmetry is to base the choice on a specific criterion. Realistically, though, such a criterion is usually at best only an approximate reflection of some vague notion of 'goodness'. Hence, it seems prudent to check that a design, selected in this fashion, performs reasonably well in other respects, relative to other possible designs."

Consider, for example, the criteria of D- and E-optimality. Using the criterion of D-optimality, we search for designs minimizing the determinant of the covariance matrix of the least squares estimate of β or, in geometric terms, the volume of the confidence ellipsoid for β (if the errors are normally distributed; cmp. with [17], Section IV.2.1). On the other hand, if we use the criterion of E-optimality, we minimize the maximum variance of linear combinations $c^T\beta$, where c are vectors of norm 1 or, equivalently, minimize the diameter of the confidence ellipsoid for β (cmp. with [17], Section IV.2.5).

However, the D-optimal design sometimes leads to a confidence ellipsoid of large diameter, while the E-optimal design can result in a confidence ellipsoid of extremely large volume. The situation is similar for the infinite number of possible criteria with their own statistical or geometric interpretations. In other words, the performance of designs can strongly depend on the choice of a criterion.

In accord with the problem described above, we set the following aims:

- **For a given experimental design ξ calculate the minimal efficiency of ξ with respect to all orthogonally invariant criteria,** i.e. calculate

$$\min_{\Phi \in \mathbb{O}} \mathrm{eff}\,(\xi|\Phi)$$

  This value, which we will call the $\mathbb{O}$-minimal efficiency of ξ, can be interpreted the measure of guaranteed performance of ξ under an arbitrary selection of a criterion from $\mathbb{O}$.

- **Find the design which maximizes the minimal efficiency with respect to all orthogonally invariant criteria**, i.e. find a design ξ^*, such that

$$\min_{\Phi \in \mathbb{O}} \mathrm{eff}\,(\xi^*|\Phi) \geq \min_{\Phi \in \mathbb{O}} \mathrm{eff}\,(\xi|\Phi) \ \text{ for all } \xi \in \Xi$$

  Therefore, ξ^* is the most performance-stable design under an arbitrary selection of a criterion from $\mathbb{O}$. We will call ξ^* the $\mathbb{O}$-maximin efficient design.

2.2 Main results of the thesis

In this section, we will give a survey of the main results of this work. Paralelly, we will describe the most important connections of the obtained results with known theorems from the optimal design literature.

2.2.1 Theoretical results

- We proved that the minimal efficiency of a design ξ with respect to the class of all orthogonally invariant criteria is equal to the minimal efficiency of ξ with respect to at most m criteria of E_k-optimality (**Theorem 11**). Therefore, the problem of how to calculate or bound the $\mathbb{O}$-minimal efficiency of any given design reduces to the problem of how to calculate or bound the E_k-optimal values of the model $(f, \mathfrak{X})$.

- To facilitate the identification of the E_k-optimal designs and values, we formulated necessary and sufficient conditions for E_k-optimality (**Theorem 6**). This theorem generalizes the equivalence theorems for E-optimality and T-optimality (see [19], p. 182 and p. 240).

- We showed that the universal optimality of a given design ξ, i.e. simultaneous optimality of ξ with respect to all orthogonally invariant criteria, can be verified by a direct maximization of at most m known functions over the experimental domain (**Theorem 12**). This result significantly simplifies the implict claim in Theorem 2.1. from the paper [1].

- We formulated a necessary and sufficient condition for the $\mathbb{O}$-maximin efficient designs (**Theorem 14**).

- We proved that for any k, the E_k-optimal value of the model $(f, \mathfrak{X})$ is bounded from above by the square the k-radius of the Elfving set (**Theorem 23**). This generalizes a result in the article [20] which states that the E-optimal value is equal or less than the squared radius of the sphere inscribed to the Elfving set.
- For the E_k-optimal values, we constructed upper bounds which depend only on the eigenvalues of a regular Φ_p-optimal information matrix (**Theorem 27**). This result leads to strenghtening of the bounds on E-efficiency of Φ_p-optimal designs given in Theorem 5.1 in the paper [6].
- We proved that the efficiency of any D-optimal design is at least h/m with respect to all orthogonally invariant criteria, where h is the minimal multiplicity of an eigenvalue of the D-optimal information matrix (**Theorem 32**).

2.2.2 Analysis of specific models

- We proved universal optimality of the uniform equidistant support design in the trigonometric regression model on $[0, 2\pi]$. This extends theorems concerning special subclasses of orthogonally invariant criteria (see [19], Section 9.16, and the article [25], Theorem 3.1). Moreover, we proved universal optimality of certain symmetric designs for a model with the experimental domain being a sphere in the l_p-norm, generalizing a result from the paper [4]. (**Chapter 7**)
- For the multivariate linear regression of the first degree over the unit cube, we found an analytic formula for the $\mathbb{O}$-minimal efficiency of the neighbor-vertex designs, covering all Φ_p-optimal designs constructed in the paper [3]. Moreover, we found the $\mathbb{O}$-maximin efficient design for any degree of the model. (**Chapter 8**)
- For the multivariate linear regression of the first degree with a constant term, we constructed the E- and D-optimal designs. We also calculated the $\mathbb{O}$-minimal efficiency of the E-optimal design and found bounds on the $\mathbb{O}$-minimal efficiency of the D-optimal design. (**Chapter 9**)
- For the quadratic, cubic and biquadratic regression on the interval $[-1, 1]$ we found all E_k-optimal designs and numerically computed the $\mathbb{O}$-minimal efficiency of all Φ_p-optimal designs. Moreover, we derived the $\mathbb{O}$-maximin efficient design for the quadratic regression. (**Chapter 10**)
- We constructed a method which allows us to remove the points from the experimental domain which can not support any D-optimal design measure. For a cubic polynomial regression without the intercept term we demonstrate how can increasingly large parts of the experimental domain be discarded in the process of computation of the D-optimal design. (**Chapter 11**)

Part II

THEORETICAL RESULTS

Chapter 3
ORTHOGONALLY INVARIANT CRITERIA

3.1 Orthogonal invariance and comparison of confidence ellipsoids

In this section, we will analyse the properties of the class $\mathbb{O}$ of orthogonally invariant criteria as defined in Section 1.3, with focus on isotonicity and orthogonal invariance. The main aim is to show why is the property of orthogonal invariance important for all criteria which measure quality of designs according to the size of the confidence ellipsoid for the parameter β.

Firstly, notice that the property of orthogonal invariance of a matrix function $\Phi : \mathcal{S}_+^m \to \Re$ is equivalent to the assumption that $\Phi(\mathbf{C})$ depends only on the eigenvalues of $\mathbf{C}$, i.e. if $\lambda(\mathbf{C}) = \lambda(\mathbf{D})$ for some $\mathbf{C}, \mathbf{D} \in \mathcal{S}_+^m$, then $\Phi(\mathbf{C}) = \Phi(\mathbf{D})$. This is an immediate consequence of the fact that $\Phi(\mathbf{C}) = \Phi(\operatorname{diag}\lambda(\mathbf{C}))$ for any $\mathbf{C} \in \mathcal{S}_+^m$ and an orthogonally invariant Φ. (For more properties of orthogonally invariant matrix functions, see e.g. [1], [26], [14] or [2] p. 104-108.)

In the sequel, we will show that orthogonal invariance together with isotonicity can be substituted by a single assumption of "spectral monotonicity"; more precisely:

Proposition 1 *([8]) Let $\Phi : \mathcal{S}_+^m \to [0, \infty)$. Then the following statements are equivalent:*
(i) *Φ is isotonic and orthogonally invariant.*
(ii) *For all $\mathbf{C}, \mathbf{D} \in \mathcal{S}_+^m$: If $\lambda(\mathbf{C}) \leq \lambda(\mathbf{D})$ then $\Phi(\mathbf{C}) \leq \Phi(\mathbf{D})$.*

Proof. Let $\Phi : \mathcal{S}_+^m \to [0, \infty)$ be isotonic and orthogonally invariant, and let $\lambda(\mathbf{C}) \leq \lambda(\mathbf{D})$ for some $\mathbf{C}, \mathbf{D} \in \mathcal{S}_+^m$. Then $\operatorname{diag}(\lambda(\mathbf{C})) \leq \operatorname{diag}(\lambda(\mathbf{D}))$ in Loewner ordering, thus $\Phi(\mathbf{C}) = \Phi(\operatorname{diag}\lambda(\mathbf{C})) \leq \Phi(\operatorname{diag}\lambda(\mathbf{D})) = \Phi(\mathbf{D})$. This proves the "(i)$\Rightarrow$(ii)" part of the proposition.

To prove the converse, suppose that for any $\mathbf{C}, \mathbf{D} \in \mathcal{S}_+^m$ such that $\lambda(\mathbf{C}) \leq \lambda(\mathbf{D})$, we have $\Phi(\mathbf{C}) \leq \Phi(\mathbf{D})$. If $\mathbf{C} \leq \mathbf{D}$, then from 7.7.4 (c) in [10], p. 471 we have $\lambda(\mathbf{C}) \leq \lambda(\mathbf{D})$ which implies $\Phi(\mathbf{C}) \leq \Phi(\mathbf{D})$ by the assumption. (See also [1], p. 327.) This proves isotonicity of Φ. Furthermore, if $\lambda(\mathbf{C}) = \lambda(\mathbf{D})$ then we have both $\lambda(\mathbf{C}) \leq \lambda(\mathbf{D})$ and $\lambda(\mathbf{D}) \leq \lambda(\mathbf{C})$, which means that $\Phi(\mathbf{C}) \leq \Phi(\mathbf{D}) \leq \Phi(\mathbf{C})$ entailing $\Phi(\mathbf{C}) = \Phi(\mathbf{D})$. Hence, $\Phi(\mathbf{C})$ depends only on the eigenvalues of $\mathbf{C}$, which means that Φ is orthogonally invariant.
■

The previous proposition can be geometrically formulated in terms of confidence ellipsoids, as we will explain. For $\widehat{\beta} \in \Re^m$, $c > 0$, and $\mathbf{C} \in \mathcal{S}_+^m$ let

$$\mathfrak{C}_{\widehat{\beta},c}(\mathbf{C}) = \left\{ b \in \mathfrak{R}^m : \left(b - \widehat{\beta}\right)^T \mathbf{C} \left(b - \widehat{\beta}\right) \leq c \right\}$$

If the errors are normally distributed and $D(\widehat{\beta}) \in \mathcal{S}^m_{++}$ is the covariance matrix of the least squares estimate $\widehat{\beta}$, then $\mathbf{C} = \left(D(\widehat{\beta})\right)^{-1}$ is the information matrix and $\mathfrak{C}_{\widehat{\beta},c}(\mathbf{C})$ is a confidence ellipsoid covering the true parameter β with probability $P\left[\chi^2_m \leq c\right]$ (For details, see [17] p. 79,80).

In the next proposition, a rigid-motion transformation is the composition of an orthogonal transformation and a shift by a vector.

Proposition 2 *([8]) Let $\Phi : \mathcal{S}^m_+ \to [0, \infty)$. Then the following statements are equivalent:*
(i) *Φ is isotonic and orthogonally invariant.*
(ii) *For all $\mathbf{C}, \mathbf{D} \in \mathcal{S}^m_+$: If for any $\widehat{\beta}_1, \widehat{\beta}_2 \in \mathfrak{R}^m$ and $c > 0$ there exists a rigid-motion transformation $\rho : \mathfrak{R}^m \to \mathfrak{R}^m$ such that $\rho(\mathfrak{C}_{\widehat{\beta}_1,c}(\mathbf{C})) \supseteq \mathfrak{C}_{\widehat{\beta}_2,c}(\mathbf{D})$, then $\Phi(\mathbf{C}) \leq \Phi(\mathbf{D})$.*

Proof. Proposition 2 follows from Proposition 1 once we prove that for all $\mathbf{C}, \mathbf{D} \in \mathcal{S}^m_+$ these two statements are equivalent:

(iii) For any $\widehat{\beta}_1, \widehat{\beta}_2 \in \mathfrak{R}^m$ and $c > 0$ there exists a rigid-motion transformation $\rho : \mathfrak{R}^m \to \mathfrak{R}^m$ such that $\rho(\mathfrak{C}_{\widehat{\beta}_1,c}(\mathbf{C})) \supseteq \mathfrak{C}_{\widehat{\beta}_2,c}(\mathbf{D})$;

(iv) $\lambda(\mathbf{C}) \leq \lambda(\mathbf{D})$ componentwise.

It is simple to show that for any $\mathbf{H} \in \mathcal{S}^m_+$, $\widehat{\beta}, s \in \mathfrak{R}^m$, $c > 0$ and a regular matrix $\mathbf{A}$ of type $m \times m$ we have

$$\mathbf{A} \cdot \mathfrak{C}_{\widehat{\beta},c}(\mathbf{H}) + s = \mathfrak{C}_{\mathbf{A}\widehat{\beta}+s,c}((\mathbf{A}^{-1})^T \mathbf{H} \mathbf{A}^{-1}).$$

"(iii)$\Rightarrow$(iv)" If (iii) holds then choosing $\widehat{\beta}_1 = \widehat{\beta}_2 = 0$ and $c = 1$ we see that there must exist $\delta \in \mathfrak{R}^m$ and an orthogonal matrix $\mathbf{U}$ such that for $\mathbf{Q} = \mathbf{U}\mathbf{C}\mathbf{U}^T$ we have $\mathfrak{C}_{\delta,1}(\mathbf{Q}) \supseteq \mathfrak{C}_{0,1}(\mathbf{D})$. Let $a \in \mathfrak{R}^m$, $d > 0$ and $a^T \mathbf{D} a \leq d$. Then the vectors $\frac{1}{\sqrt{d}} a$ and $-\frac{1}{\sqrt{d}} a$ are members of $\mathfrak{C}_{0,1}(\mathbf{D})$, hence they both belong to $\mathfrak{C}_{\delta,1}(\mathbf{Q})$. It follows that

$$\left(\tfrac{1}{\sqrt{d}} a - \delta\right)^T \mathbf{Q} \left(\tfrac{1}{\sqrt{d}} a - \delta\right) \leq 1 \text{ as well as } \left(-\tfrac{1}{\sqrt{d}} a - \delta\right)^T \mathbf{Q} \left(-\tfrac{1}{\sqrt{d}} a - \delta\right) \leq 1.$$

Summing up these two inequalities we obtain $\frac{1}{d} a^T \mathbf{Q} a + \delta^T \mathbf{Q} \delta \leq 1$. Because $\mathbf{Q} \in \mathcal{S}^m_+$ we have $\delta^T \mathbf{Q} \delta \geq 0$, thence $a^T \mathbf{Q} a \leq d$. This clearly implies that for any $a \in \mathfrak{R}^m$ we have $a^T \mathbf{Q} a \leq a^T \mathbf{D} a$ and consequently $\mathbf{Q} \leq \mathbf{D}$ in Loewner ordering. Therefore $\lambda(\mathbf{C}) = \lambda(\mathbf{Q}) \leq \lambda(\mathbf{D})$, where the inequality follows from 7.7.4 (c) in [10].

"(iii)$\Leftarrow$(iv)" Let (iv) hold, $\mathbf{D} = \mathbf{V} \operatorname{diag}(\lambda(\mathbf{D})) \mathbf{V}^T$ and $\mathbf{C} = \mathbf{R} \operatorname{diag}(\lambda(\mathbf{C})) \mathbf{R}^T$ for some orthogonal matrices $\mathbf{V}$, $\mathbf{R}$. Let $\widehat{\beta}_1, \widehat{\beta}_2 \in \mathfrak{R}^m$ and $c > 0$ be arbitrary. Let ρ be the rigid-motion transformation which is defined by the formula

$$\rho(\cdot) = \mathbf{U} \times (\cdot) + r, \text{ where } \mathbf{U} = \mathbf{V}\mathbf{R}^T,\ r = \widehat{\beta}_2 - \mathbf{U}\widehat{\beta}_1$$

Evidently, $\lambda(\mathbf{C}) \leq \lambda(\mathbf{D})$ implies that for all $\widehat{\beta} \in \mathfrak{R}^m$: $\mathfrak{C}_{\widehat{\beta},c}(\operatorname{diag}(\lambda(\mathbf{C}))) \supseteq \mathfrak{C}_{\widehat{\beta},c}(\operatorname{diag}(\lambda(\mathbf{D})))$. Therefore

$$\rho(\mathfrak{C}_{\widehat{\beta}_1,c}(\mathbf{C})) = \mathfrak{C}_{\mathbf{U}\widehat{\beta}_1+r,c}(\mathbf{UCU}^T) = \mathfrak{C}_{\widehat{\beta}_2,c}(\mathbf{V}\,\mathrm{diag}\,(\lambda\,(\mathbf{C}))\,\mathbf{V}^T) =$$
$$= \mathbf{V}\cdot\mathfrak{C}_{\mathbf{V}^T\widehat{\beta}_2,c}(\mathrm{diag}\,(\lambda\,(\mathbf{C}))) \supseteq \mathbf{V}\cdot\mathfrak{C}_{\mathbf{V}^T\widehat{\beta}_2,c}(\mathrm{diag}\,(\lambda\,(\mathbf{D}))) = \mathfrak{C}_{\widehat{\beta}_2,c}(\mathbf{D})$$

■

The previous proposition can be roughly formulated as follows. Suppose that we consider a confidence ellipsoid $\mathfrak{C}_1$ to be "equally large or larger" than a confidence ellipsoid $\mathfrak{C}_2$, if $\mathfrak{C}_1$ can be shifted and orthogonally rotated to cover $\mathfrak{C}_2$. Moreover, define a partial ordering $\sqsubseteq$ comparing the amout of information contained in information matrices $\mathbf{C}$, $\mathbf{D}$ as $\mathbf{C} \sqsubseteq \mathbf{D}$ iff the confidence ellipsoid corresponding to $\mathbf{C}$ will certainly be equally large or larger than the confidence ellipsoid corresponding to $\mathbf{D}$. Then Proposition 2 means that, for a matrix function $\Phi : \mathcal{S}_+^m \to [0,\infty)$, the properties of Loewner isotonicity and orthogonal invariance can be substituted by the assumption of monotonicity with respect to the ordering $\sqsubseteq$.

3.2 Criteria of E_k-optimality

In this section we begin the study of a class of criteria having an essential importance for the entire work.

For $k \in \{1,...,m\}$, let $\widetilde{\Phi}_{E_k}(\mathbf{A})$ be the sum of the k smallest eigenvalues of $\mathbf{A} \in \mathcal{S}^m$, i.e.

$$\widetilde{\Phi}_{E_k} : \mathcal{S}^m \to (-\infty,\infty)\,,\ \widetilde{\Phi}_{E_k}(\mathbf{A}) = \sum_{i=1}^{k} \lambda_i(\mathbf{A})$$

The restriction of the function $\widetilde{\Phi}_{E_k}$ onto $\mathcal{S}_+^m$ is the criterion Φ_{E_k} of E_k-optimality defined in Section 1.3.

Evidently, the functions Φ_{E_k} are orthogonally invariant. Proposition 1 implies that these functions are also isotonic. Furthermore, positive homogeneity and upper semicontinuity are clear (upper semicontinuity is a consequence of continuity of the functions $\lambda_i : \mathcal{S}^m \to \mathfrak{R}$ themselves; cmp. e.g. [10] p. 540). Moreover, for any $\mathbf{C} \in \mathcal{S}_+^m$ we have

$$\Phi_{E_k}(\mathbf{C}) = \min\nolimits_{\mathbf{U}\in\mathcal{U}_{m,k}} \mathrm{tr}\,\mathbf{U}^T\mathbf{CU}$$

where $\mathcal{U}_{m,k}$ is the set of all matrices $\mathbf{U}$ of type $m \times k$, such that $\mathbf{U}^T\mathbf{U} = \mathbf{I}_k$ (the theorem of Ky Fan; see e.g. [10] p. 191). It follows that Φ_{E_k} is a minimum of linear functions, which entails concavity of Φ_{E_k} (see also [14], [16]). Consequently, we obtained

Proposition 3 *([8]) For any $k \in \{1,...,m\}$, the function $\Phi_{E_k} : \mathcal{S}_+^m \to [0,\infty)$ is an orthogonally invariant criterion.*

Notice that criteria Φ_{E_k} are not strictly concave (i.e. we can have more than one E_k-optimal information matrix) and, with the exception of Φ_{E_1}, they can be positive for a singular information matrix (as is the case, for instance, in the polynomial regression model analyzed in Chapter 10).

The functions $\widetilde{\Phi}_{E_k}$ are not differentiable everywhere on $\mathcal{S}^m$, with the exception of the linear function $\widetilde{\Phi}_{E_m}$. Nonetheless, it is possible to find the subdifferential $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ of the function $\widetilde{\Phi}_{E_k}$ in any fixed $\mathbf{A} \in \mathcal{S}^m$, which is the set of all subgradients of $\widetilde{\Phi}_{E_k}$ in $\mathbf{A}$ (see [22] p. 308 or [21]; notice that the trace of a product of two matrices corresponds to the scalar product):

$$\partial\widetilde{\Phi}_{E_k}(\mathbf{A}) = \left\{\mathbf{Y} \in \mathcal{S}^m : \widetilde{\Phi}_{E_k}(\mathbf{B}) \leq \widetilde{\Phi}_{E_k}(\mathbf{A}) + \operatorname{tr}\left((\mathbf{B} - \mathbf{A})\,\mathbf{Y}\right) \text{ for all } \mathbf{B} \in \mathcal{S}^m\right\}.$$

The following proposition is in all important aspects equal to a claim published in [14] (see also [16]).

Proposition 4 *Let $\mathbf{A} \in \mathcal{S}^m$, and let $\lambda(\mathbf{A}) = \lambda = (\lambda_1, ..., \lambda_m)^T$. Then $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ is the set of all matrices $\mathbf{U}\operatorname{diag}(\gamma)\,\mathbf{U}^T$, where the orthogonal matrix $\mathbf{U}$ satisfies $\mathbf{A} = \mathbf{U}\operatorname{diag}(\lambda)\,\mathbf{U}^T$, and the vector $\gamma = (\gamma_1, ..., \gamma_m)^T$ satisfies: $\gamma_i \in [0,1]$ for all $i = 1, ..., m$, $\gamma_i = 1$ if $\lambda_i < \lambda_k$, $\gamma_i = 0$ if $\lambda_i > \lambda_k$, and $\sum_{i=1}^m \gamma_i = k$.*

In the case of $\lambda_k(\mathbf{A})$ being *strictly* less than $\lambda_{k+1}(\mathbf{A})$, the subdifferential $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ contains elements $\sum_{i=1}^k u_i u_i^T$, where $\mathbf{A}u_i = \lambda_i(\mathbf{A})u_i$, $\langle u_i, u_j\rangle = \delta_{ij}$ (Kronecker delta) for $i, j = 1, ..., k$. It is easy to see that for any choice of the vectors u_i, the sum $\sum_{i=1}^k u_i u_i^T$ is a unique matrix: the orthogonal projector on the linear space generated by the eigenvectors of $\mathbf{A}$ corresponding to the k smallest eigenvalues. That is, in this case the function $\widetilde{\Phi}_{E_k}$ is differentiable in $\mathbf{A}$, and the gradient is the matrix of orthogonal projection.

If $\lambda_k(\mathbf{A}) = \lambda_{k+1}(\mathbf{A})$, then the compact and convex set $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ contains a full continuum of matrices, not all of which must be projectors, but projectors do play an important role also in the general subdifferential $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$. (By $\|\mathbf{Q}\|_F$ we denote the Frobenius norm of $\mathbf{Q} \in \mathcal{S}^m$: $\|\mathbf{Q}\|_F = \sqrt{\operatorname{tr}(\mathbf{Q}^2)}$.)

Proposition 5 *Let $\mathbf{A} \in \mathcal{S}^m$, and $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{A})$. Then $\operatorname{tr}(\mathbf{Y}) = k$ and $\|\mathbf{Y}\|_F \leq \sqrt{k}$. Moreover, the next three statements are equivalent:*
(i) *$\mathbf{Y}$ is an extreme point of $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$.*
(ii) *$\mathbf{Y}$ is an orthogonal projector which projects on a k-dimensional subspace of $\mathfrak{R}^m$.*
(iii) *$\|\mathbf{Y}\|_F = \sqrt{k}$.*

Proof. For $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ we have $\operatorname{tr}(\mathbf{Y}) = k$ and $\|\mathbf{Y}\|_F \leq \sqrt{k}$ which directly follows from Proposition 4. We shall prove "(i)$\Leftrightarrow$(ii)$\Leftrightarrow$(iii)" in the second part of the proposition.

"(i)$\Rightarrow$(ii)": For $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ we can assume that $\mathbf{Y} = \mathbf{U}\operatorname{diag}(\gamma)\,\mathbf{U}^T$, where $\mathbf{U} \in \mathcal{U}_{m,m}$ and $\gamma \in [0,1]^m$ satisfy the conditions given by Proposition 4.

Suppose that $\mathbf{Y}$ is *not* an orthogonal projector, which means that $\gamma \notin \{0,1\}^m$. As $\sum_{i=1}^m \gamma_i$ is a natural number (k), there must exist at least two indices $1 \leq i_1 < i_2 \leq m$ such that the components $\gamma_{i_1}, \gamma_{i_2} \in [\varepsilon, 1-\varepsilon]$ for some $\varepsilon \in (0, 1/2]$. Obviously, i_1, i_2 must be such that $\lambda_{i_1}(\mathbf{A}) = \lambda_{i_2}(\mathbf{A}) = \lambda_k(\mathbf{A})$. Take the m-dimensional vectors

$\gamma^{(1)}, \gamma^{(2)}$ having the components same as γ with these exceptions: $\gamma_{i_1}^{(1)} = \gamma_{i_1} - \varepsilon$, $\gamma_{i_2}^{(1)} = \gamma_{i_2} + \varepsilon$, $\gamma_{i_1}^{(2)} = \gamma_{i_1} + \varepsilon$ and $\gamma_{i_2}^{(2)} = \gamma_{i_2} - \varepsilon$. It is straightforward to check that the vectors $\gamma^{(1)}, \gamma^{(2)}$ are chosen such that both $\mathbf{Y}_1 = \mathbf{U}\,\mathrm{diag}\left(\gamma^{(1)}\right)\mathbf{U}^T$ and $\mathbf{Y}_2 = \mathbf{U}\,\mathrm{diag}\left(\gamma^{(2)}\right)\mathbf{U}^T$ belong to $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$, and that $\frac{1}{2}\mathbf{Y}_1 + \frac{1}{2}\mathbf{Y}_2 = \mathbf{Y}$. Therefore, $\mathbf{Y}$ is *not* an extreme point of $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$.

We can close the proof of "(i)⇒(ii)" noticing that any member of $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ has trace equal to k, which means that any projector from $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ must project on a k-dimensional space (the trace of an idempotent matrix is its rank).

"(ii)⇒(iii)": If $\mathbf{Y}$ is an orthogonal projector on a k-dimensional space, then $\mathbf{Y}$ is idempotent with trace k, hence $\|\mathbf{Y}\|_F^2 = \mathrm{tr}\left(\mathbf{Y}^2\right) = \mathrm{tr}\left(\mathbf{Y}\right) = k$, which implies (iii).

"(iii)⇒(i)": If $\|\mathbf{Y}\|_F = \sqrt{k}$, then $\mathbf{Y}$ is clearly an extreme point of the ball $\mathcal{B} = \left\{\mathbf{Q} \in \mathcal{S}^m : \|\mathbf{Q}\|_F \leq \sqrt{k}\right\}$, and because $\partial\widetilde{\Phi}_{E_k}(\mathbf{A}) \subseteq \mathcal{B}$ we obtain (i).
■

Thus, the Minkowski Theorem (see e.g. [22] p. 167 or [2] p.68) entails that $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$ is a convex hull of the set of all orthogonal projectors contained in $\partial\widetilde{\Phi}_{E_k}(\mathbf{A})$. (We remark that a convex combination of two orthogonal projectors does not have to be an orthogonal projector itself.)

3.3 Equivalence theorem for E_k-optimality

Using $\partial\widetilde{\Phi}_{E_k}$, we can formulate a characterization of E_k-optimal designs, i.e. an "equivalence theorem" for E_k-optimality in the general model $(f, \mathfrak{X})$.

Theorem 6 *([8]) Let $\zeta \in \Xi$ and let $\lambda = (\lambda_1, ..., \lambda_m)^T = \lambda(\mathbf{M}(\zeta))$. Then the next three statements are equivalent:*
(i) *ζ is E_k-optimal for the model $(f, \mathfrak{X})$.*
(ii) *$\Phi_{E_k}(\mathbf{M}(\zeta)) = \max_{x\in\mathfrak{X}} f^T(x)\mathbf{Y}f(x)$ for some $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{M}(\zeta))$.*
(iii) *$\Phi_{E_k}(\mathbf{M}(\zeta)) = \max_{x\in\mathfrak{X}} f^T(x)\mathbf{Y}f(x)$ for some $\mathbf{Y} \in \mathcal{S}_+^m$ such that $\mathrm{tr}(\mathbf{Y}) = k$, $\mathbf{Y} \leq \mathbf{I}_m$.*

Proof. A well known theorem from convex analysis (see e.g. [22] part 7.4. or [21]) implies that $\mathbf{M} = \mathbf{M}(\zeta)$ maximizes $\widetilde{\Phi}_{E_k}$ (hence also Φ_{E_k}) on $\mathcal{M}$ if and only if there exists $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{M})$, such that $\mathrm{tr}(\mathbf{NY}) \leq \mathrm{tr}(\mathbf{MY})$ for all $\mathbf{N} \in \mathcal{M}$, resp. iff $\sup_{\mathbf{N}\in\mathcal{M}} \mathrm{tr}(\mathbf{NY}) = \mathrm{tr}(\mathbf{MY})$. But

$$\begin{aligned} \sup\nolimits_{\mathbf{N}\in\mathcal{M}} \mathrm{tr}(\mathbf{NY}) &= \sup\nolimits_{\xi\in\Xi} \mathrm{tr}(\textstyle\sum_{\xi(x)>0} \xi(x) f(x) f^T(x)\mathbf{Y}) = \\ &= \sup\nolimits_{\xi\in\Xi} \textstyle\sum_{\xi(x)>0} \xi(x) f^T(x)\mathbf{Y}f(x) = \max_{x\in\mathfrak{X}} f^T(x)\mathbf{Y}f(x) \end{aligned}$$

Also, for any choice $\mathbf{Y} = \mathbf{U}\,\mathrm{diag}(\gamma)\,\mathbf{U}^T$ where $\mathbf{U}$, γ are given in Proposition 4, we have $\mathrm{tr}(\mathbf{MY}) = \mathrm{tr}(\mathrm{diag}(\lambda)\,\mathrm{diag}(\gamma)) = \Phi_{E_k}(\mathbf{M})$. This proves (i)⇔(ii).

Next, the implication (ii)⇒(iii) follows from Proposition 4, as for any $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{M})$ we have $\mathrm{tr}(\mathbf{Y}) = k$, and $\lambda_i(\mathbf{Y}) \in [0, 1]$ giving $\mathbf{Y} \leq \mathbf{I}_m$.

We will prove (iii)⇒(ii) by simply showing that the matrix $\mathbf{Y}$ from (iii) is a subgradient of $\widetilde{\Phi}_{E_k}$ in $\mathbf{M} = \mathbf{M}(\zeta)$. Let (iii) hold. Obviously

$$\begin{gathered}\operatorname{tr}(\mathbf{MY}) = \operatorname{tr}(\textstyle\sum_{\zeta(x)>0} \zeta\,(x)\, f(x) f^T(x)\mathbf{Y}) = \\ = \textstyle\sum_{\zeta(x)>0} \zeta\,(x)\, f^T(x)\mathbf{Y} f(x) \leq \max\limits_{x\in\mathfrak{X}} f^T(x)\mathbf{Y} f(x) = \Phi_{E_k}(\mathbf{M}).\end{gathered}$$

For any $\mathbf{B} \in \mathcal{S}^m$ we thus have $\widetilde{\Phi}_{E_k}(\mathbf{M}) + \operatorname{tr}((\mathbf{B}-\mathbf{M})\,\mathbf{Y}) \geq \operatorname{tr}(\mathbf{BY})$. Moreover from Theorem 3.4 in [16] it follows that:

$$\widetilde{\Phi}_{E_k}(\mathbf{B}) = \min\left\{\operatorname{tr}(\mathbf{BH}) : \mathbf{H} \in \mathcal{S}_+^m, \mathbf{H} \leq \mathbf{I}_m, \operatorname{tr}(\mathbf{H}) = k\right\}.$$

Hence $\operatorname{tr}(\mathbf{BY}) \geq \widetilde{\Phi}_{E_k}(\mathbf{B})$, which entails $\widetilde{\Phi}_{E_k}(\mathbf{M}) + \operatorname{tr}((\mathbf{B}-\mathbf{M})\,\mathbf{Y}) \geq \widetilde{\Phi}_{E_k}(\mathbf{B})$. By the definition of subgradient, this means that $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{M})$.

■

Notice that the previous theorem gives us a generalization of the equivalence theorem for E-optimality in the form of [19], p. 182. The equivalence theorem for T-optimality [19], p. 240 is a direct consequence as well.

According to the discussion above, Theorem 6 provides an easy test of E_k-optimality for those designs ζ, that $\mathbf{M} = \mathbf{M}(\zeta)$ has $\lambda_k(\mathbf{M}) < \lambda_{k+1}(\mathbf{M})$, i.e. if $\widetilde{\Phi}_{E_k}$ is differentiable in $\mathbf{M}$. In such a case we only need to check that

$$\Phi_{E_k}(\mathbf{M}) = \max_{x\in\mathfrak{X}} \textstyle\sum_{i=1}^k \left(f^T(x)u_i\right)^2$$

where $u_1, ..., u_k$ are (arbitrary) orthonormal eigenvectors corresponding to the eigenvalues $\lambda_1(\mathbf{M}), ..., \lambda_k(\mathbf{M})$.

If $\widetilde{\Phi}_{E_k}$ is not differentiable in $\mathbf{M}$, that is if $\partial\widetilde{\Phi}_{E_k}(\mathbf{M})$ contains more than one element, then Theorem 6 can still be applicable. The reason is that $\partial\widetilde{\Phi}_{E_k}(\mathbf{M})$ is a convex set (generated by a known set of projectors; see Proposition 5) and for all $x \in \mathfrak{X}$ the function $f^T(x)\,(\cdot)\, f(x) : \mathcal{S}^m \to \mathfrak{R}$ is linear, therefore $\max_{x\in\mathfrak{X}} f^T(x)\,(\cdot)\, f(x)$ is a finite convex function. Nevertheless, finding the appropriate subgradient can be a hard convex-optimization problem itself.

The efficiency of designs with respect to criteria of E_k-optimality is of particular interest in the following parts of this work.

Theorem 7 *Let $\xi \in \Xi$, and let $k \in \{1, ..., m\}$. Then*

$$\operatorname{eff}(\xi|\Phi_{E_k}) \geq \frac{\Phi_{E_k}(\mathbf{M}(\xi))}{\max\limits_{x\in\mathfrak{X}} f^T(x)\mathbf{Y} f(x)} \text{ for any } \mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{M}(\xi))$$

Proof. Let $\xi \in \Xi$, $1 \leq k \leq m$, ζ_k^* be an E_k-optimal design, and let $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{M}(\xi))$. From the definition of subgradient we have

$$\Phi_{E_k}(\mathbf{M}(\zeta_k^*)) \leq \Phi_{E_k}(\mathbf{M}(\xi)) + \operatorname{tr}((\mathbf{M}(\zeta_k^*) - \mathbf{M}(\xi))\,\mathbf{Y})$$

In the same time, we can show that $\operatorname{tr}(\mathbf{M}(\zeta_k^*)\,\mathbf{Y}) \leq \max\limits_{x\in\mathfrak{X}} f^T(x)\mathbf{Y} f(x)$ and $\Phi_{E_k}(\mathbf{M}(\xi)) = \operatorname{tr}(\mathbf{M}(\xi)\,\mathbf{Y})$ similarly as in the proof of "(i)⇔(ii)" in Theorem 6. Combining these three facts we obtain $\Phi_{E_k}(\mathbf{M}(\zeta_k^*)) \leq \max_{x\in\mathfrak{X}} f^T(x)\mathbf{Y}f(x)$. The theorem now follows from the definition of efficiency. (Notice also that we obtained $\max_{x\in\mathfrak{X}} f^T(x)\mathbf{Y}f(x) > 0$.)

■

If $\widetilde{\Phi}_{E_k}$ is not differentiable in $\mathbf{M}(\xi)$, the strongest bound on the E_k-efficiency of $\xi \in \Xi$ based on Theorem 7 assumes that we find the minimum of $\max_{x\in\mathfrak{X}} f^T(x)\mathbf{Y}f(x)$ for all subgradients $\mathbf{Y}$. Here we can encounter similar problems as in the case that we need to verify E_k-optimality of ζ (see the discussion after Theorem 6). Fortunately, we will be able to avoid these difficulties in computation of bounds on the $\mathbb{O}$-minimal efficiency of a design defined and analyzed in the next section, esp. Theorem 11. In this respect, the following auxiliary result will be important:

Proposition 8 *For $k \in \{1,...,m\}$ and $\xi \in \Xi$ define $v_\xi(k) = \Phi_{E_k}(\mathbf{M}(\xi))$ and $v_\xi(0) = 0$. Let $v_\xi(\cdot) : [0,m] \to [0,\infty)$ be the piecewise-linear function interpolating nodes $(0, v_\xi(0)), ..., (m, v_\xi(m))$, which means that for $x \in [0,m)$*

$$v_\xi(x) = (1-(x-\lfloor x\rfloor))v_\xi(\lfloor x\rfloor) + (x-\lfloor x\rfloor)v_\xi(\lfloor x\rfloor + 1)$$

Consider the function $v(\cdot) : [0,m] \to [0,\infty)$ defined by

$$v(x) = \sup_{\xi\in\Xi} v_\xi(x) \text{ for } x \in [0,m]$$

Then v is an increasing convex function.

Proof. The only nontrivial step is to show that v is convex. This will follow once we prove that for any fixed ξ the function v_ξ is convex, since a pointwise supremum of convex functions is again a convex function (see e.g. [22], p. 35; notice also that the functions v_ξ are bounded from above by the E_m-optimal value.) The case $m = 1$ is trivial. Let $m > 1$. Clearly, to prove convexity of the piecewise linear function v_ξ it suffices to show that $v_\xi(k+1) - v_\xi(k) \geq v_\xi(k) - v_\xi(k-1)$ for all $k = 1, ..., m-1$. But this inequality is equivalent to $\lambda_{k+1}(\mathbf{M}(\xi)) \geq \lambda_k(\mathbf{M}(\xi))$.

■

For the E_k-optimal values of an m-dimensional model $(f, \mathfrak{X})$ we will use the notation $v_{f,\mathfrak{X}}(k)$, or simply $v(k)$ if the model in consideration is clear from the context. Notice that for an integer k, the symbol $v(k)$ from the previous theorem is consistent with our notation of the E_k-optimal values.

Chapter 4

MINIMAL EFFICIENCY OF DESIGNS UNDER THE CLASS OF ORTHOGONALLY INVARIANT INFORMATION CRITERIA

4.1 The $\mathbb{O}$-minimal efficiency of designs

In this chapter we will prove the main theoretical results of this work. We will show that, as far as the problem of minimal efficiency (and universal optimality) is concerned, we can restrict our attention from the uncountable class $\mathbb{O}$ to the finite subset of criteria of E_k-optimality.

Suppose that $\xi, \zeta \in \Xi$ are designs such that $\mathbf{M}(\xi) \in \mathcal{S}^m_{++}$, and let $\Phi \in \mathbb{O}$. Let us define the relative Φ-efficiency of ξ with respect to ζ in the form

$$\mathrm{eff}(\xi : \zeta|\Phi) = \Phi(\mathbf{M}(\xi)) / \Phi(\mathbf{M}(\zeta))$$

where $c/0 = \infty$ for $c > 0$. The efficiency $\mathrm{eff}(\xi : \zeta|\Phi)$ can thus be intuitively interpreted as the proportion of the information gained by the design ξ compared to ζ.

Theorem 9 *([8]) Let $\xi, \zeta \in \Xi$, $\mathbf{M}(\xi) \in \mathcal{S}^m_{++}$. Then*

$$\inf_{\Phi \in \mathbb{O}} \mathrm{eff}(\xi : \zeta|\Phi) = \min_{k=1,\dots,m} \mathrm{eff}(\xi : \zeta|\Phi_{E_k})$$

Proof. Recall that an $m \times m$ matrix $\mathbf{S}$ is said to be doubly stochastic, if it has nonnegative entries and each column and row is summing to one. An $m \times m$ matrix $\mathbf{P}$ is a permutation matrix, if each row and column contains exactly one element 1, and $m-1$ elements 0. Evidently, there are $m!$ such matrices.

Let $\mathfrak{R}^m_+$, and $\mathfrak{R}^m_\leq$ denote the set of all m-dimensional vectors with nonnegative components (the nonnegative orthant), resp. the set of all vectors with components in a nondecreasing order. Let $x = (x_1, ..., x_m)^T, y = (y_1, ..., y_m)^T \in \mathfrak{R}^m_\leq$. If $\sum_{i=1}^k x_i \geq \sum_{i=1}^k y_i$ for $k = 1, ..., m-1$, and $\sum_{i=1}^m x_i = \sum_{i=1}^m y_i$, then we will say that x majorizes y, and denote this fact by $x \succeq y$. (We use this notion as defined e.g. in [10] p.192, cf. also with [19], p.144-5.)

In the proof, we will use the following theorems:

1. (Birkhoff theorem, see e.g. [10] p. 527) An $m \times m$ matrix $\mathbf{S}$ is doubly stochastic if and only if $\mathbf{S}$ is a convex combination of permutation matrices.

2. (Hardy-Littlewood-Pólya theorem; see e.g. [10] p. 197) If $x, y \in \mathfrak{R}^m_+ \cap \mathfrak{R}^m_\leq$, then $x \succeq y$ if and only if $x = \mathbf{S}y$ for some doubly stochastic matrix $\mathbf{S}$.

Evidently, the inequality $\inf_{\Phi \in \mathbb{O}} \mathrm{eff}(\xi : \zeta|\Phi) \leq \min_{k=1,\dots,m} \mathrm{eff}(\xi : \zeta|\Phi_{E_k})$ is clear because $\Phi_{E_k} \in \mathbb{O}$. We will prove the converse inequality.

Denote $l = \lambda(\mathbf{M}(\xi))$ and $g = \lambda(\mathbf{M}(\zeta))$. Define $0^{-1} = \infty$, $\infty^{-1} = 0$, and set

$$\delta = \min_{k=1,\dots,m} \mathrm{eff}(\xi : \zeta | \Phi_{E_k}) = \min_{k=1,\dots,m} \left(\sum_{i=1}^{k} l_i\right) \left(\sum_{i=1}^{k} g_i\right)^{-1},$$
$$g_m^* = \delta^{-1} \left(\sum_{i=1}^{m} l_i\right) - \sum_{i=1}^{m-1} g_i, \text{ and } g^* = (g_1, \dots, g_{m-1}, g_m^*)^T$$

As $\delta \leq (\sum_{i=1}^{m} l_i)(\sum_{i=1}^{m} g_i)^{-1}$, we have $g_m^* \geq g_m$, hence $g^* \geq g$ and $g^* \in \mathfrak{R}_+^m \cap \mathfrak{R}_\leq^m$. Moreover, $\delta^{-1} \sum_{i=1}^{k} l_i \geq \sum_{i=1}^{k} g_i$ for $k = 1, \dots, m-1$, and $\delta^{-1} \sum_{i=1}^{m} l_i = \left(\sum_{i=1}^{m-1} g_i\right) + g_m^*$, which implies $\delta^{-1} l \succeq g^*$. Therefore, by the Hardy-Littlewood-Pólya theorem there exists a doubly stochastic matrix $\mathbf{S}$ of the type $m \times m$, such that $\delta^{-1} l = \mathbf{S} g^*$. Because the elements of $\mathbf{S}$, as well as the coordinates of g and g^* are nonnegative, the inequality $g^* \geq g$ implies $\mathbf{S} g^* \geq \mathbf{S} g$, therefore $\delta^{-1} l \geq \mathbf{S} g$. Next, from the Birkhoff theorem we know that $\mathbf{S} = \sum_{j=1}^{m!} \alpha_j \mathbf{P}_j$, where $\mathbf{P}_j$ is the j-th permutation matrix, $\alpha_j \in [0,1]$ for $j = 1, \dots, m!$, and $\sum_{j=1}^{m!} \alpha_j = 1$.

Let $\Phi \in \mathbb{O}$. For any permutation matrix $\mathbf{P}_j$ it holds that $\Phi(\mathrm{diag}\, \mathbf{P}_j g) = \Phi(\mathrm{diag}\, g)$, since Φ is orthogonally invariant. Hence, the orthogonal invariance, concavity, isotonicity, and homogeneity of Φ imply:

$$\Phi(\mathbf{M}(\zeta)) = \Phi(\mathrm{diag}\, g) = \sum_{j=1}^{m!} \alpha_j (\Phi(\mathrm{diag}\, g)) = \sum_{j=1}^{m!} \alpha_j (\Phi(\mathrm{diag}\, \mathbf{P}_j g)) \leq$$
$$\leq \Phi\left(\mathrm{diag}\left(\sum_{j=1}^{m!} \alpha_j \mathbf{P}_j g\right)\right) = \Phi(\mathrm{diag}(\mathbf{S} g)) \leq \Phi(\mathrm{diag}(\delta^{-1} l)) = \delta^{-1} \Phi(\mathbf{M}(\xi))$$

Therefore $\mathrm{eff}(\xi : \zeta | \Phi) = \Phi(\mathbf{M}(\xi)) / \Phi(\mathbf{M}(\zeta)) \geq \delta$ which concludes the proof of Theorem 9.

■

An important consequence of Theorem 9 is that it gives us a method how to compute the minimal (absolute) efficiency with respect to $\mathbb{O}$ for any design. From the previous theorem we immediately obtain:

Theorem 10 *([8]) Let $\xi \in \Xi$ be any design. Then*

$$\inf_{\Phi \in \mathbb{O}} \mathrm{eff}(\xi | \Phi) = \min_{k=1,\dots,m} \mathrm{eff}(\xi | \Phi_{E_k})$$

Hence, the minimal efficiency with respect to the uncountable set of all orthogonally invariant criteria is simply the minimal efficiency with respect to the set of criteria Φ_{E_k}, which numbers only m elements. In other words, once we computed the model-specific E_k-optimal values $v(k)$, we can directly calculate the minimal efficiency for any design ξ as

$$\inf_{\Phi \in \mathbb{O}} \mathrm{eff}(\xi | \Phi) = \min_{k=1,\dots,m} \{\Phi_{E_k}(\mathbf{M}(\xi)) / v(k)\}$$

We will call the value $\inf_{\Phi \in \mathbb{O}} \mathrm{eff}(\xi | \Phi)$ also the $\mathbb{O}$-minimal efficiency of ξ and denote it briefly by $\mathrm{mineff}(\xi | \mathbb{O})$, or $\mathrm{mineff}_{f,\mathfrak{X}}(\xi | \mathbb{O})$ if we feel the need to emphasize the dependence on the model $(f, \mathfrak{X})$.

Surprisingly, in the previous theorem we can safely disregard the E_k-efficiency of ξ for any such k, for which $\widetilde{\Phi}_{E_k}$ is not differentiable in $\mathbf{M}(\xi)$. We will formalize this claim in the following important strengthening of Theorem 10, including the entailed bounds on the $\mathbb{O}$-minimal efficiency.

Let ξ be a design. Define the set

$$\mathfrak{D}(\xi) = \{k \in \{1, ..., m-1\} : \lambda_k(\mathbf{M}(\xi)) < \lambda_{k+1}(\mathbf{M}(\xi))\} \cup \{m\}$$

The set $\mathfrak{D}(\xi) = \mathfrak{D}_{f,\mathfrak{X}}(\xi)$ corresponds to those indices $k \in \{1, ..., m\}$, such that $\widetilde{\Phi}_{E_k}$ is differentiable in $\mathbf{M}(\xi)$. (See the remarks after Proposition 4.)

Theorem 11 *Let $\xi \in \Xi$ be any design. Then*

$$\text{mineff}(\xi|\mathbb{O}) = \min_{k \in \mathfrak{D}(\xi)} \text{eff}(\xi|\Phi_{E_k})$$

Moreover, let $\mathbf{M}(\xi) = \mathbf{U}\,\text{diag}\,\lambda(\mathbf{M}(\xi))\,\mathbf{U}^T$ for some $\mathbf{U} = (u_1, ..., u_m) \in \mathcal{U}_{m,m}$. Define matrices $\mathbf{U}_k = (u_1, ..., u_k)$ for $k = 1, ..., m$. Then

$$\text{mineff}(\xi|\mathbb{O}) \geq \min_{k \in \mathfrak{D}(\xi)} \frac{\Phi_{E_k}(\mathbf{M}(\xi))}{\max_{x \in \mathfrak{X}} \|\mathbf{U}_k^T f(x)\|^2}$$

Proof. For the first part of the theorem it suffices to prove that if $s \in \{1, ..., m-1\}$ and $s \notin \mathfrak{D}(\xi)$, then $\text{eff}(\xi|\Phi_{E_s}) \geq \text{eff}(\xi|\Phi_{E_k})$ for some $k \in \{1, ..., m\}$, $k \neq s$, in view of Theorem 10.

Consider the functions v_ξ and v from Proposition 8. If $s \notin \mathfrak{D}(\xi)$ then $\lambda_s(\mathbf{M}(\xi)) = \lambda_{s+1}(\mathbf{M}(\xi))$, therefore $v_\xi(s-1) + v_\xi(s+1) = 2v_\xi(s)$. Next, v is convex which means $v(s-1) + v(s+1) \geq 2v(s)$. Consequently, for any $s \notin \mathfrak{D}(\xi)$ we can write:

$$\text{eff}(\xi|\Phi_{E_s}) = \frac{v_\xi(s)}{v(s)} \geq \frac{v_\xi(s-1) + v_\xi(s+1)}{v(s-1) + v(s+1)}$$

Hence, if $s = 1$ then $v_\xi(s-1) = v(s-1) = 0$ implies:

$$\text{eff}(\xi|\Phi_{E_s}) = \text{eff}(\xi|\Phi_{E_{s+1}})$$

If $s > 1$ we can use a decomposition to a convex combination to obtain:

$$\text{eff}(\xi|\Phi_{E_s}) \geq \frac{v(s-1)}{v(s-1)+v(s+1)} \frac{v_\xi(s-1)}{v(s-1)} + \frac{v(s+1)}{v(s-1)+v(s+1)} \frac{v_\xi(s+1)}{v(s+1)} \geq$$

$$\geq \min\left\{\frac{v_\xi(s-1)}{v(s-1)}, \frac{v_\xi(s+1)}{v(s+1)}\right\} = \min\left\{\text{eff}(\xi|\Phi_{E_{s-1}}), \text{eff}(\xi|\Phi_{E_{s+1}})\right\}$$

The first part is thus proved.

The proof of the second part of the theorem uses the first part, Theorem 7, and the fact that, in the case of differentiability, the gradient of Φ_{E_k} in $\mathbf{M}(\xi)$ is $\mathbf{U}_k\mathbf{U}_k^T$ (Proposition 4). Consequently, for (the only one) $\mathbf{Y} \in \partial\widetilde{\Phi}_{E_k}(\mathbf{M}(\xi))$ we have $\max_{x \in \mathfrak{X}} f^T(x)\mathbf{Y}f(x) = \max_{x \in \mathfrak{X}} \left\|\mathbf{U}_k^T f(x)\right\|^2$.

■

4.2 Equivalence theorem for universal optimality

It turns out that designs optimal with respect to all orthogonally invariant criteria do exist in some special models. An example is the equispaced support design in the trigonometric regression on the full circle or a sufficiently symmetric uniform design on an m-dimensional sphere (see Chapter 7 for these and some other examples).

An immediate consequence of Theorem 10 is that a design ξ is optimal with respect to all orthogonally invariant criteria (in other words: ξ is "universally" optimal for the class $\mathbb{O}$) if and only if ξ is Φ_{E_k}-optimal for all $k = 1, ..., m$. We point out that this condition characterizing universally optimal designs is same as the one obtained by Bondar for a somewhat different (yet related) class of criteria; see [1] for details. However, we can formulate a much more explicit condition of how to verify universal optimality, as we will show in the sequel.

To prove that a design ξ is universally optimal, that is Φ_{E_k}-optimal for all $k = 1, ..., m$, we can use the equivalence theorem for E_k-optimality. However, this theorem is difficult to apply for the cases when Φ_{E_k} is not differentiable in $\mathbf{M}(\xi)$. Nevertheless, one consequence of Theorem 11 is that we only need to check E_k-optimality for the "easy" values of k, circumventing all difficulties with nondifferentiability. In the following claim we use the set $\mathfrak{D}(\xi)$ and matrices $\mathbf{U}_1, ..., \mathbf{U}_m$ consisting of eigenvectors of $\mathbf{M}(\xi)$ exactly as in Theorem 11.

Theorem 12 *Let $\xi \in \Xi$. Then the following three statements are equivalent.*
(i) *ξ is optimal with respect to all orthogonally invariant criteria.*
(ii) *ξ is E_k-optimal for all $k \in \mathfrak{D}(\xi)$.*
(iii) *$\Phi_{E_k}(\mathbf{M}(\xi)) = \max_{x \in \mathfrak{X}} \left\| \mathbf{U}_k^T f(x) \right\|^2$ for all $k \in \mathfrak{D}(\xi)$.*

Proof. Follows directly from Theorem 11. ■

Although universal optimality is based on nondifferentiable criteria, the previous theorem allows us to check universal optimality in a very similar way as the equivalence theorems for differentiable criteria - by a simple maximization of known functions over the compact set $\mathfrak{X}$.

4.3 $\mathbb{O}$-maximin efficient designs

The results of Section 4.1 entail a natural question: If the model in consideration does not admit a universally optimal design, are we able to find the design with maximum possible $\mathbb{O}$-minimal efficiency?

Consider the matrix function

$$\widetilde{\Phi}_{\mathbb{O}} : \mathcal{S}^m \to (-\infty, \infty); \ \widetilde{\Phi}_{\mathbb{O}}(\mathbf{A}) = \min_{k=1,...,m} \frac{\widetilde{\Phi}_{E_k}(\mathbf{A})}{v(k)},$$

where $v(k)$ is the E_k-optimal value, $k = 1, ..., m$. Clearly, the function $\Phi_{\mathbb{O}}$, defined as the restriction of $\widetilde{\Phi}_{\mathbb{O}}$ onto $\mathcal{S}_+^m$, is an orthogonally invariant criterion and, in accord with Theorem 10, we can consider it to be the criterion of $\mathbb{O}$-minimal efficiency for the model $(f, \mathfrak{X})$. Therefore, the $\Phi_{\mathbb{O}}$-optimal design can be called the maximin efficient design with respect to $\mathbb{O}$ (shortly $\mathbb{O}$-maximin efficient design).

As $\widetilde{\Phi}_{\mathbb{O}}$ is a finite minimum of concave functions, it is not difficult to find the subdifferential of $\widetilde{\Phi}_{\mathbb{O}}$, and consequently formulate an equivalence theorem for the $\mathbb{O}$-maximin efficient design. The next proposition follows from a general formula giving the subgradient of a minimum of concave functions which can be found e.g. in [2] p.47. (Cf. also [22] p.223.)

Proposition 13 *([8]) Let* $\mathbf{A} \in \mathcal{S}^m$ *and let*

$$\mathfrak{I} = \left\{k \in \{1, ..., m\} : \widetilde{\Phi}_{E_k}(\mathbf{A})/v(k) = \widetilde{\Phi}_{\mathbb{O}}(\mathbf{A})\right\}$$

Then subdifferential of $\widetilde{\Phi}_{\mathbb{O}}$ *in* $\mathbf{A}$ *is the set*

$$\partial\widetilde{\Phi}_{\mathbb{O}}(\mathbf{A}) = \bigcup\left\{\sum_{k\in\mathfrak{I}} \frac{\alpha_k}{v(k)} \partial\widetilde{\Phi}_{E_k}(\mathbf{A}) : \sum_{k\in\mathfrak{I}} \alpha_k = 1, \text{ and } \alpha_k \geq 0 \text{ for } k \in \mathfrak{I}\right\}$$

Theorem 14 *([8]) A design* ξ *is maximin efficient with respect to* $\mathbb{O}$ *if and only if there exists* $\mathbf{Y} \in \partial\widetilde{\Phi}_{\mathbb{O}}(\mathbf{M}(\xi))$*, such that* $\Phi_{\mathbb{O}}(\mathbf{M}(\xi)) = \max_{x\in\mathfrak{X}} f^T(x)\mathbf{Y}f(x)$.

The proof of the previous theorem is similar to the proof of (i)$\Leftrightarrow$(ii) in Theorem 6 and is therefore omitted. Notice that if $\mathbf{M}(\xi)$ is a point of nondifferentiability of $\widetilde{\Phi}_{\mathbb{O}}$, then $\partial\widetilde{\Phi}_{\mathbb{O}}(\mathbf{M}(\xi))$ possibly contains a continuum of subgradients, and the previous theorem does not give us a method how to choose the right one for the equivalence determining optimality. We also remark that the previous theorem can be formulated in terms of directional derivatives of $\widetilde{\Phi}_{E_k}$, similarly as in [15]. Nevertheless, both approaches are essentially same, and they suffer analogous disadvantages.

To illustrate the concept of $\mathbb{O}$-maximin efficiency on an example, we will determine the maximin efficient designs (which are not universally optimal) for multivariate linear regression models in Section 8.3 and for the quadratic regression on $[-1, 1]$ in Section 10.3.

Very often, it is difficult to find the exact E_k-optimal values which are necessary to *begin* the search for an $\mathbb{O}$-maximin efficient design. (For example in Chapter 9 we were not able to find the E_k-optimal values exactly, which precludes further search for the $\mathbb{O}$-maximin efficient design.) Hence, an analytic calculation of the $\mathbb{O}$-maximin efficient design can be a very hard problem. Therefore, a numerical algorithm determining the E_k-optimal values and, accordingly, computing the $\mathbb{O}$-maximin efficient design, would be a very useful addition to the theory developed in this work. Although our preliminary considerations suggest that such an algorithm can indeed be constructed (see e.g. [31], or [30] for some potentially useful methods), we refrained from developing the complicated numerical methods in this work. The only numerical construction of efficiency-robust (but, in general, *not* $\mathbb{O}$-maximin efficient) designs is hinted in the next section; the reason is its appealing simplicity.

4.4 Efficiency robust designs based on linear programming

Let ζ_k^* be a known E_k-optimal design for $k = 1, ..., m$. As mentioned above, knowledge of the designs ζ_k^* does not automatically mean that we can find an $\mathbb{O}$-maximin efficient design. Nevertheless, we can use them to construct a design with $\mathbb{O}$-minimal efficiency at least (but possibly much more than) $1/m$.

Consider a vector $w \in \mathfrak{R}_+^m$; $\sum_{i=1}^m w_i = 1$ of weights and the convex combination of the E_k-optimal designs given by

$$\overline{\zeta}_w = \sum_{i=1}^m w_i \zeta_i^*$$

From concavity of functions Φ_{E_k} we obtain

$$\operatorname{mineff}\left(\overline{\zeta}_w|\mathbb{O}\right) = \min_{k=1,...,m}\left(\operatorname{eff}\left(\sum_{i=1}^m w_i\zeta_i^*|\Phi_{E_k}\right)\right) \geq \min_{k=1,...,m}\left(\sum_{i=1}^m w_i \operatorname{eff}(\zeta_i^*|\Phi_{E_k})\right)$$

For any fixed k, the sum $\sum_{i=1}^m w_i \operatorname{eff}(\zeta_i^*|\Phi_{E_k})$ contains the term $w_k \operatorname{eff}(\zeta_k^*|\Phi_{E_k}) = w_k$, which clearly implies

$$\operatorname{mineff}\left(\overline{\zeta}_w|\mathbb{O}\right) \geq \min\{w_1, ..., w_m\}$$

Setting $w_1 = ... = w_m = 1/m$ we see that the average of the E_k-optimal designs satisfies $\operatorname{mineff}\left(\overline{\zeta}_w|\mathbb{O}\right) \geq 1/m$. (We will show that any D-optimal design has this property as well; see Corollary 32.)

Nonetheless, we can go further and try to find the vector of weights

$$w^* = \operatorname{argmax}_w \left\{\min_{k=1,...,m}\left(\sum_{i=1}^m w_i \operatorname{eff}(\zeta_i^*|\Phi_{E_k})\right)\right\}$$

such that for w^* the lower bound on the $\mathbb{O}$-minimal efficiency of $\overline{\zeta}_w$ is maximized. Clearly, this requires maximization of a polyhedral concave function over an m-dimensional simplex of weights, which is equivalent to the following problem of linear programming:

maximize y subject to

$$\begin{pmatrix} \operatorname{eff}(\zeta_1^*|\Phi_{E_1}) & \cdots & \operatorname{eff}(\zeta_m^*|\Phi_{E_1}) & -1 & 0 & \cdots & 0 & -1 \\ \operatorname{eff}(\zeta_1^*|\Phi_{E_2}) & \cdots & \operatorname{eff}(\zeta_m^*|\Phi_{E_2}) & 0 & -1 & \cdots & 0 & -1 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \operatorname{eff}(\zeta_1^*|\Phi_{E_m}) & \cdots & \operatorname{eff}(\zeta_m^*|\Phi_{E_m}) & 0 & 0 & \cdots & -1 & -1 \\ 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \begin{pmatrix} w_1 \\ \vdots \\ w_m \\ \delta_1 \\ \vdots \\ \delta_m \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

$(w_1, ..., w_m, \delta_1, ..., \delta_m, y)^T \in \mathfrak{R}_+^{2m+1}$

To solve this problem, we can use standard algorithms as the simplex method. (See e.g. [28] for a book on linear programming which can be of particular interest for a statistician.) Because the number of parameters m of a regression model is usually small, it is also possible to simply compute all individual extreme points of the compact polyhedral feasible set and find the optimum by a direct comparison of their last component y. Geometry of linear programming entails that the number of the extreme points with nonzero y is at most $\binom{2m}{m}$ and the computation of them requires solving at most $\binom{2m}{m}$ systems of $m+1$ independent linear equations with $m+1$ unknowns.

We will exemplify this method on the quadratic regression model in Section 10.3 by calculating the design $\overline{\zeta}_{w^*}$ and comparing its performance with the known $\mathbb{O}$-maximin efficient design.

Chapter 5

BOUNDS ON THE E_K-EFFICIENCY AND THE $\mathbb{O}$-MINIMAL EFFICIENCY BASED ON ORTHOGONAL SUBMODELS

5.1 Orthogonal submodels and the Poincaré separation theorem

In this chapter we prove that the E_k-optimal values of an m-dimensional model $(f, \mathfrak{X})$ can be bounded from below as well as from above by the optimal values of orthogonal submodels of $(f, \mathfrak{X})$. We will show that some of the obtained bounds admit an interpretation as the k-radii of the Elfving set, which generalizes a known result about E-optimality. Using the k-radii of the Elfving set, we can formulate a necessary and sufficient condition for universal optimality under the class of orthogonally invariant criteria.

Let $1 \leq k \leq m$ be two natural numbers. Recall that $\mathcal{U}_{m,k}$ denotes the set of all matrices $\mathbf{U}$ of type $m \times k$ such that $\mathbf{U}^T\mathbf{U} = \mathbf{I}_k$, i.e. $\mathcal{U}_{m,k}$ is the set of all matrices $(u_1, ..., u_k)$ where $u_1, ..., u_k \in \mathfrak{R}^m$ form an orthonormal system of vectors.

A k-dimensional model $(g, \mathfrak{X})$ will be called an orthogonal submodel of $(f, \mathfrak{X})$ if $g = \mathbf{U}^T f$ for some $\mathbf{U} \in \mathcal{U}_{m,k}$. That is, an orthogonal submodel of $(f, \mathfrak{X})$ is any model which consists of $k \leq m$ components of $(f, \mathfrak{X})$, or of some orthogonal reparametrization of $(f, \mathfrak{X})$. Notice that the relation of being an orthogonal submodel is transitive, which means that if $(h, \mathfrak{X})$ is an orthogonal submodel of $(g, \mathfrak{X})$ and if $(g, \mathfrak{X})$ is an orthogonal submodel of $(f, \mathfrak{X})$ then $(h, \mathfrak{X})$ is an orthogonal submodel of $(f, \mathfrak{X})$. This follows from the fact that if $1 \leq r \leq k \leq m$, $\mathbf{U} \in \mathcal{U}_{m,k}$ and $\mathbf{V} \in \mathcal{U}_{k,r}$, then $\mathbf{UV} \in \mathcal{U}_{m,r}$.

Let $\left(\mathbf{U}^T f, \mathfrak{X}\right)$ be an r-dimensional orthogonal submodel of an m-dimensional model $(f, \mathfrak{X})$, where $\mathbf{U} \in \mathcal{U}_{m,r}$. Then

$$\mathbf{M}_{\mathbf{U}^T f, \mathfrak{X}}(\xi) = \mathbf{U}^T \mathbf{M}_{f,\mathfrak{X}}(\xi)\mathbf{U} \text{ for all } \xi \in \Xi_{\mathfrak{X}}$$

$$\mathcal{M}_{\mathbf{U}^T f, \mathfrak{X}} = \mathbf{U}^T \mathcal{M}_{f,\mathfrak{X}} \mathbf{U}$$

This explains the need for analysis of the relations between the eigenvalues of matrices $\mathbf{M} \in \mathcal{S}_+^m$ and $\mathbf{U}^T\mathbf{M}\mathbf{U} \in \mathcal{S}_+^r$. The main theoretical tool which we will use is the Poincaré separation theorem (see e.g. [10] p. 190). For the purpose of this chapter, we formulate the theorem in the following form.

Lemma 15 *Let $r, m \in \mathfrak{N}$, $1 \leq r \leq m$ and let $\mathbf{M} \in \mathcal{S}_+^m$, $\mathbf{U} \in \mathcal{U}_{m,r}$, $\mathbf{N} = \mathbf{U}^T\mathbf{M}\mathbf{U}$. Then for all $k = 1, ..., r$*

$$\lambda_k(\mathbf{M}) \leq \lambda_k(\mathbf{N}) \leq \lambda_{k+m-r}(\mathbf{M})$$

To give a more intuitive description of the previous lemma, consider the special case $r = m-1$, $m > 1$. Then $\mathbf{N} = \mathbf{U}^T\mathbf{M}\mathbf{U} \in \mathcal{S}_+^{m-1}$ and the claim of Lemma 15 can be visualized by the following scheme, where $a \to b$ denotes $a \leq b$.

$$\begin{array}{ccccccccc}
\lambda_1(\mathbf{M}) & \to & \lambda_2(\mathbf{M}) & \to & \lambda_3(\mathbf{M}) & \cdots & \lambda_{m-1}(\mathbf{M}) & \to & \lambda_m(\mathbf{M}) \\
\downarrow & \nearrow & \downarrow & \nearrow & \downarrow & \cdots & \downarrow & \nearrow & \\
\lambda_1(\mathbf{N}) & \to & \lambda_2(\mathbf{N}) & \to & \lambda_3(\mathbf{N}) & \cdots & \lambda_{m-1}(\mathbf{N}) & &
\end{array}$$

As a direct application of the Poincaré separation theorem we obtain:

Proposition 16 *Let $r, m \in \mathfrak{N}$, $1 \leq r \leq m$ and let $\mathbf{M} \in \mathcal{S}_+^m$, $\mathbf{U} \in \mathcal{U}_{m,r}$, $\mathbf{N} = \mathbf{U}^T\mathbf{M}\mathbf{U}$. Then*

$$\begin{array}{ll}
\Phi_{E_k}(\mathbf{M}) \leq \Phi_{E_k}(\mathbf{N}) & \text{if } k \in \{1, ..., r\} \\
\Phi_{E_k}(\mathbf{M}) \geq \Phi_{E_{k-m+r}}(\mathbf{N}) + \Phi_{E_{m-r}}(\mathbf{M}) & \text{if } k \in \{m-r+1, ..., m\}\,,\ r < m
\end{array}$$

The first corollary pertaining to the problem of E_k-optimality is Theorem 17. Recall that by $v_{g,\mathfrak{X}}(k)$ we denote the E_k-optimal value of a model $(g, \mathfrak{X})$.

Theorem 17 *Let $1 \leq k \leq m$ and let $(f, \mathfrak{X})$ be an m-dimensional model. Suppose that*

$$\Phi_{E_k}\left(\mathbf{M}_{f,\mathfrak{X}}(\zeta)\right) \geq v_{g,\mathfrak{X}}(k)$$

for some design $\zeta \in \Xi_{\mathfrak{X}}$ and an r-dimensional orthogonal submodel $(g, \mathfrak{X})$ of the model $(f, \mathfrak{X})$, where $k \leq r \leq m$. Then the following statements hold:
(i) *The design ζ is E_k-optimal for the model $(f, \mathfrak{X})$;*
(ii) *Any design which is E_k-optimal for $(f, \mathfrak{X})$ is also E_k-optimal for $(g, \mathfrak{X})$.*

Proof. Let $1 \leq k \leq m$, $\zeta \in \Xi_{\mathfrak{X}}$ and let $\Phi_{E_k}\left(\mathbf{M}_{f,\mathfrak{X}}(\zeta)\right) = v_{\mathbf{U}^T f,\mathfrak{X}}(k)$ for some $\mathbf{U} \in \mathcal{U}_{m,r}$ such that $k \leq r \leq m$. Let $\zeta_k^* \in \Xi_{\mathfrak{X}}$ be any E_k-optimal design for the model $(f, \mathfrak{X})$. From the assumption, Proposition 16, and from the fact that $\mathbf{U}^T\mathbf{M}_{f,\mathfrak{X}}(\zeta_k^*)\mathbf{U} = \mathbf{M}_{\mathbf{U}^T f,\mathfrak{X}}(\zeta_k^*)$ we obtain

$$\begin{array}{l}
v_{\mathbf{U}^T f,\mathfrak{X}}(k) = \Phi_{E_k}\left(\mathbf{M}_{f,\mathfrak{X}}(\zeta)\right) \leq v_{f,\mathfrak{X}}(k) = \Phi_{E_k}\left(\mathbf{M}_{f,\mathfrak{X}}(\zeta_k^*)\right) \leq \\
\leq \Phi_{E_k}\left(\mathbf{U}^T\mathbf{M}_{f,\mathfrak{X}}(\zeta_k^*)\mathbf{U}\right) = \Phi_{E_k}\left(\mathbf{M}_{\mathbf{U}^T f,\mathfrak{X}}(\zeta_k^*)\right) \leq v_{\mathbf{U}^T f,\mathfrak{X}}(k)
\end{array}$$

Therefore $\Phi_{E_k}\left(\mathbf{M}_{f,\mathfrak{X}}(\zeta)\right) = v_{f,\mathfrak{X}}(k)$ which implies (i) and $\Phi_{E_k}\left(\mathbf{M}_{\mathbf{U}^T f,\mathfrak{X}}(\zeta_k^*)\right) = v_{\mathbf{U}^T f,\mathfrak{X}}(k)$ which entails (ii).
■

Thus, a suitable orthogonal submodel $(g, \mathfrak{X})$ of the model $(f, \mathfrak{X})$ can be used to prove E_k-optimality of a given design $\xi \in \Xi_{\mathfrak{X}}$. In this view, Theorem 17 is a sufficient condition on E_k-optimality. Moreover, it can also help us determine *all* E_k-optimal designs of the model $(f, \mathfrak{X})$ in the sense that the only candidates on the E_k-optimal designs of $(f, \mathfrak{X})$ are the E_k-optimal designs of $(g, \mathfrak{X})$. We remark that the model $(g, \mathfrak{X})$ can have greatly reduced dimension or exhibit some easy to analyse symmetries, which directly yield the E_k-optimal values $v_{g,\mathfrak{X}}(k)$. The use of Theorem 17 is demonstrated in the proofs of Theorems 47 and 56.

5.2 Bounds on E_k-optimal values determined by orthogonal submodels

Proposition 16 immediately gives us bounds on the Φ_{E_k}-optimal values of $(f, \mathfrak{X})$.

Proposition 18 *Let $r, m \in \mathfrak{N}$, $m > 1$, $1 \leq r < m$. Let $(f, \mathfrak{X})$ be an m-dimensional model and $\mathbf{U} \in \mathcal{U}_{m,r}$. Then*

$$\begin{array}{ll} v_{f,\mathfrak{X}}(k) \leq v_{\mathbf{U}^T f,\mathfrak{X}}(k) & \text{if } k \in \{1, ..., r\} \\ v_{f,\mathfrak{X}}(k) \geq v_{\mathbf{U}^T f,\mathfrak{X}}(k - m + r) & \text{if } k \in \{m - r + 1, ..., m\} \end{array}$$

The particularly important *upper* bound on $v_{f,\mathfrak{X}}(k)$ given by the previous theorem can be concisely restated as follows: the E_k-optimal value of the model $(f, \mathfrak{X})$ is bounded from above by the E_k-optimal value of any of its orthogonal submodels.

Suppose now that $(f_1, \mathfrak{X}), (f_2, \mathfrak{X}), ...$ is a sequence of models such that $(f_i, \mathfrak{X})$ is an i-dimensional orthogonal submodel of $(f_{i+1}, \mathfrak{X})$ for $i = 1, 2, ...$ Proposition 18 implies that the relations between the values $v_{f_i,\mathfrak{X}}(k)$ can be visualized by a "lattice" of bounds depicted below. (Compare this diagram with the exact E_k-optimal values for the successive degrees models of spring balance weighing in Section 8.2 and for the polynomial models in Section 10.1.)

$$\begin{array}{ccccccccc}
v_{f_1,\mathfrak{X}}(1) & \leftarrow & v_{f_2,\mathfrak{X}}(1) & \leftarrow & v_{f_3,\mathfrak{X}}(1) & \leftarrow & v_{f_4,\mathfrak{X}}(1) & \leftarrow & \cdots \\
 & \searrow & \downarrow & \searrow & \downarrow & \searrow & \downarrow & \searrow & \cdots \\
 & & v_{f_2,\mathfrak{X}}(2) & \leftarrow & v_{f_3,\mathfrak{X}}(2) & \leftarrow & v_{f_4,\mathfrak{X}}(2) & \leftarrow & \cdots \\
 & & & \searrow & \downarrow & \searrow & \downarrow & \searrow & \cdots \\
 & & & & v_{f_3,\mathfrak{X}}(3) & \leftarrow & v_{f_4,\mathfrak{X}}(3) & \leftarrow & \cdots \\
 & & & & & \searrow & \downarrow & \searrow & \cdots \\
 & & & & & & v_{f_4,\mathfrak{X}}(4) & \leftarrow & \cdots \\
 & & & & & & & \searrow & \cdots \\
 & & & & & & & & \cdots
\end{array}$$

Taking the set of *all* orthogonal submodels of $(f, \mathfrak{X})$ into account, we obtain the following chain of bounds on $v_{f,\mathfrak{X}}(k)$ from above.

Theorem 19 *Let $(f, \mathfrak{X})$ be an m-dimensional model, $m > 1$, and let $k \in \{1, ..., m - 1\}$. Then*

$$v_{f,\mathfrak{X}}(k) \leq \inf_{\mathbf{U} \in \mathcal{U}_{m,m-1}} v_{\mathbf{U}^T f,\mathfrak{X}}(k) \leq ... \leq \inf_{\mathbf{U} \in \mathcal{U}_{m,k}} v_{\mathbf{U}^T f,\mathfrak{X}}(k)$$

Moreover, let $\mathbf{M}$ be an E_k-optimal information matrix for $(f, \mathfrak{X})$ and let $\lambda_k(\mathbf{M}) < \lambda_s(\mathbf{M})$ for some $s \in \{k + 1, ..., m\}$. Let $u_1, ..., u_{s-1}$ be a sequence of orthonormal eigenvectors of $\mathbf{M}$ corresponding to $\lambda_1(\mathbf{M}), ..., \lambda_{s-1}(\mathbf{M})$. Then $v_{f,\mathfrak{X}}(k) = v_{\mathbf{U}^T f,\mathfrak{X}}(k)$ for $\mathbf{U} = (u_1, ..., u_{s-1}) \in \mathcal{U}_{m,s-1}$.

Proof.

Let $r \in \{k + 1, .., m\}$. Take $\mathbf{U}_1 \in \mathcal{U}_{m,r-1}$ and any vector $u \in \mathfrak{R}^m$, $\|u\| = 1$ such that u is orthogonal to all columns of $\mathbf{U}_1$. Clearly, $\mathbf{U}_0 = (\mathbf{U}_1, u) \in \mathcal{U}_{m,r}$. Therefore $\left(\mathbf{U}_1^T f, \mathfrak{X}\right)$ is an orthogonal submodel of $\left(\mathbf{U}_0^T f, \mathfrak{X}\right)$, which means that $v_{\mathbf{U}_0^T f,\mathfrak{X}}(k) \leq v_{\mathbf{U}_1^T f,\mathfrak{X}}(k)$ by Proposition 18. Since $\mathbf{U}_1 \in \mathcal{U}_{m,r-1}$ was arbitrary, we obtained

$$\inf_{\mathbf{U}\in\mathcal{U}_{m,r}} v_{\mathbf{U}^T f,\mathfrak{X}}(k) \leq \inf_{\mathbf{U}\in\mathcal{U}_{m,r-1}} v_{\mathbf{U}^T f,\mathfrak{X}}(k)$$

This implies the first part of the theorem.

To prove the second part, let $\mathbf{M}$, s, and $\mathbf{U} = (u_1, ..., u_{s-1}) \in \mathcal{U}_{m,s-1}$ be as described in the statement of the theorem, and let $\lambda = \lambda(\mathbf{M})$. As $\mathbf{M}$ is assumed to be E_k-optimal, Proposition 4 and the part "(i)⇔(ii)" of Theorem 6 imply that there exist coefficients $\gamma_1, .., \gamma_{s-1} \in [0, 1]$, such that $\sum_{i=1}^{s-1} \gamma_i = k$, next $\gamma_i = 1$ if $\lambda_i < \lambda_k$, $\gamma_i = 0$ if $\lambda_i > \lambda_k$ and

$$\Phi_{E_k}(\mathbf{M}) = \max_{x\in\mathfrak{X}} f^T(x) \left(\sum_{i=1}^{s-1} \gamma_i u_i u_i^T\right) f(x) = \\ \max_{x\in\mathfrak{X}} (\mathbf{U}^T f)^T(x) \operatorname{diag}(\gamma_1, .., \gamma_{s-1})(\mathbf{U}^T f)(x)$$

Moreover, $\mathbf{U}^T\mathbf{M}\mathbf{U} = \operatorname{diag}(\lambda_1, ..., \lambda_{s-1})$ which implies $\Phi_{E_k}\left(\mathbf{U}^T\mathbf{M}\mathbf{U}\right) = \Phi_{E_k}(\mathbf{M})$, therefore

$$\Phi_{E_k}\left(\mathbf{U}^T\mathbf{M}\mathbf{U}\right) = \max_{x\in\mathfrak{X}} (\mathbf{U}^T f)^T(x) \operatorname{diag}(\gamma_1, .., \gamma_{s-1})(\mathbf{U}^T f)(x)$$

On the other hand $\operatorname{tr}(\operatorname{diag}(\gamma_1, .., \gamma_{s-1})) = k$ and $\operatorname{diag}(\gamma_1, .., \gamma_{s-1}) \leq \mathbf{I}_m$, which means that $\mathbf{U}^T\mathbf{M}\mathbf{U}$ is E_k-optimal for $\left(\mathbf{U}^T f, \mathfrak{X}\right)$ by Theorem 6, part "(i)⇔(iii)". Consequently

$$v_{\mathbf{U}^T f,\mathfrak{X}}(k) = \Phi_{E_k}\left(\mathbf{U}^T\mathbf{M}\mathbf{U}\right) = \Phi_{E_k}(\mathbf{M}) = v_{f,\mathfrak{X}}(k).$$

■

The previous theorem extends the use of Theorem 17 such that it gives us a condition under which there indeed does exist an orthogonal submodel of $(f, \mathfrak{X})$ with the same E_k-optimal value as the suppermodel.

For example, assume that we are able to rule out the possibility that the information matrix of an E-optimal design ξ is proportional to the identity matrix. By Theorem 19, the design ξ is among the E-optimal designs of some $m-1$ dimensional orthogonal submodel of $(f, \mathfrak{X})$. This submodel is the one which is "minimal" in the sense that it has the minimal E-optimal value, from all $m-1$ dimensional orthogonal submodels of $(f, \mathfrak{X})$.

For completeness, we will also formulate a counterpart of Theorem 19 giving us a sequence of lower bounds on the E_k-optimal values.

Theorem 20 *Let $(f, \mathfrak{X})$ be an m-dimensional model, $m > 1$, and let $k \in \{2, ..., m\}$. Then*

$$v_{f,\mathfrak{X}}(k) \geq \sup_{\mathbf{U}\in\mathcal{U}_{m,m-1}} v_{\mathbf{U}^T f,\mathfrak{X}}(k-1) \geq ... \geq \sup_{\mathbf{U}\in\mathcal{U}_{m,m-k+1}} v_{\mathbf{U}^T f,\mathfrak{X}}(1)$$

Moreover, let $\mathbf{M}$ be an E_k-optimal information matrix for $(f, \mathfrak{X})$ and let $\lambda_1(\mathbf{M}) = \lambda_2(\mathbf{M}) = ... = \lambda_s(\mathbf{M}) = 0$ for some $s \in \{1, ..., k-1\}$. Let $u_{s+1}, ..., u_m$ be a sequence of orthonormal eigenvectors of $\mathbf{M}$ corresponding to $\lambda_{s+1}(\mathbf{M}), ..., \lambda_m(\mathbf{M})$. Then $v_{f,\mathfrak{X}}(k) = v_{\mathbf{U}^T f,\mathfrak{X}}(k-s)$ for $\mathbf{U} = (u_{s+1}, ..., u_m) \in \mathcal{U}_{m,m-s}$.

Proof. Let $r \in \{1, ..., k-1\}$. Take any $\mathbf{U}_1 \in \mathcal{U}_{m,m-r}$ and choose a vector $u \in \mathfrak{R}^m$, $\|u\| = 1$ such that u is orthogonal to all columns of $\mathbf{U}_1$. We have $\mathbf{U}_0 = (\mathbf{U}_1, u) \in \mathcal{U}_{m,m-r+1}$, and $\left(\mathbf{U}_1^T f, \mathfrak{X}\right)$ is an orthogonal submodel of $\left(\mathbf{U}_0^T f, \mathfrak{X}\right)$, hence $v_{\mathbf{U}_0^T f,\mathfrak{X}}(k-r+1) \geq v_{\mathbf{U}_1^T f,\mathfrak{X}}(k-r)$ by Proposition 18. As $\mathbf{U}_1$ was an arbitrary member of $\mathcal{U}_{m,m-r}$, we obtain

$$\sup{}_{\mathbf{U}\in\mathcal{U}_{m,m-r+1}} v_{\mathbf{U}^T f,\mathfrak{X}}(k-r+1) \geq \sup{}_{\mathbf{U}\in\mathcal{U}_{m,m-r}} v_{\mathbf{U}^T f,\mathfrak{X}}(k-r)$$

This proves the first part of the theorem. For the second part, suppose that $\mathbf{M}$, s, and $\mathbf{U} = (u_{s+1}, ..., u_m) \in \mathcal{U}_{m,m-s}$ satisfy assumptions of the premise. Clearly $\mathbf{U}^T\mathbf{M}\mathbf{U} = \mathrm{diag}\left(\lambda_{s+1}(\mathbf{M}), ..., \lambda_m(\mathbf{M})\right)$ hence

$$v_{f,\mathfrak{X}}(k) = \textstyle\sum_{i=s+1}^{k} \lambda_i(\mathbf{M}) = \Phi_{E_{k-s}}(\mathbf{U}^T\mathbf{M}\mathbf{U}) \leq v_{\mathbf{U}^T f,\mathfrak{X}}(k-s)$$

By Proposition 18 we have $v_{f,\mathfrak{X}}(k) \geq v_{\mathbf{U}^T f,\mathfrak{X}}(k-s)$ and consequently $v_{f,\mathfrak{X}}(k) = v_{\mathbf{U}^T f,\mathfrak{X}}(k-s)$.

■

For $k > 1$, the E_k-optimal information matrix for the model $(f, \mathfrak{X})$ can be singular, in which case the E_k-optimal value is equal to the E_{k-s}-optimal value for some orthogonal submodel of dimension $s < m$. This is the case in the polynomial regression model; see Section 10.1. Nevertheless, there are special models, where any E_k-optimal information matrix is regular (for $k < m$) and $v_{f,\mathfrak{X}}(k)$ is strictly greater than the largest lower bound from Theorem 20. An example is the regression model on a sphere in $\mathfrak{R}^m$ centered in origin (Section 7.1).

5.3 Elfving set geometry of the bounds on E_k-optimal values

Many properties of the model $(f, \mathfrak{X})$, which are interesting from the perspective of optimal experimental design, can be geometrically analyzed using the Elfving set defined in Section 1.1 (see e.g. [17], [19], [18], [4], or [5]) .

The most important use of the Elfving set is its geometric characterization of c-optimal designs as given by the Elfving theorem (see [17], p. 71, or [19], p. 50). From the large number of relations between the compact set $\mathfrak{E}_{f,\mathfrak{X}}$ and optimal designs for $(f, \mathfrak{X})$, we select those which are most relevant for the problem of E_k-optimality. For a design $\xi \in \Xi_{\mathfrak{X}}$ let $\mathrm{supp}\,(\xi) = \{x \in \mathfrak{X}; \xi\,(x) > 0\}$ be the support of ξ.

Proposition 21 *Let Φ be an orthogonally invariant information criterion.*
(i) *For any model $(f, \mathfrak{X})$ there exists a Φ-optimal design $\xi^* \in \Xi_{\mathfrak{X}}$, such that $f(\mathrm{supp}\,(\xi))$ is a subset of the set of extreme points of $\mathfrak{E}_{f,\mathfrak{X}}$.*
(ii) *Let $(f_1, \mathfrak{X}_1)$ and $(f_2, \mathfrak{X}_2)$ be models of the same dimension and let $\mathfrak{E}_{f_1,\mathfrak{X}_1} \subseteq \mathfrak{E}_{f_2,\mathfrak{X}_2}$. Then the Φ-optimal value of $(f_1, \mathfrak{X}_1)$ is less or equal to the Φ-optimal value of $(f_2, \mathfrak{X}_2)$.*

Proof. The part (i) follows from Proposition III.7. in [17] or Theorem 8.5. in [19]. We will prove (ii).

Let $\Phi : \mathcal{S}_+^m \to [0, \infty)$, $\Phi \in \mathbb{O}$. Firstly, we will show that if two m-dimensional models $(f_1, \mathfrak{X})$ and $(f_2, \mathfrak{X})$ have the same Elfving sets, then they have the same Φ-optimal values (denoted by $v_{f_1,\mathfrak{X}}(\Phi)$, resp. $v_{f_2,\mathfrak{X}}(\Phi)$).

Suppose that $\mathfrak{E}_{f_1,\mathfrak{X}} = \mathfrak{E}_{f_2,\mathfrak{X}}$. Let $\xi^* \in \Xi_{\mathfrak{X}}$ be a design which is Φ-optimal for $(f_1, \mathfrak{X})$ and which is chosen in accord with the part (i) of this theorem, i.e. such that $\mathrm{supp}\,(\xi^*)$ is a subset of the set of extreme points of $\mathfrak{E}_{f_1,\mathfrak{X}}$. Let $x \in \mathrm{supp}\,(\xi^*)$. Since $f_1(x)$ is an extreme point of $\mathfrak{E}_{f_1,\mathfrak{X}}$, and because the Elfving sets are assumed to be equal, the point $f_1(x)$ is also extreme for $\mathfrak{E}_{f_2,\mathfrak{X}}$. This entails that $f_1(x) = f_2(x^*)$ or $f_1(x) = -f_2(x^*)$ for some $x^* \in \mathfrak{X}$, hence $f_1(x)f_1^T(x) = f_2(x^*)f_2^T(x^*)$. Therefore, $\mathbf{M}_{f_1,\mathfrak{X}}(\xi^*) = \sum_{x\in X;\xi^*(x)>0} \xi^*(x)f_1(x)f_1^T(x)$ can be expressed as a convex combination of matrices of type $f_2(x^*)f_2^T(x^*)$, where $x^* \in \mathfrak{X}$. We thus obtained $\mathbf{M}_{f_1,\mathfrak{X}}(\xi^*) \in \mathcal{M}_{f_2,\mathfrak{X}}$, thence $v_{f_1,\mathfrak{X}}(\Phi) \leq v_{f_2,\mathfrak{X}}(\Phi)$. Using the same argument we can show that $v_{f_2,\mathfrak{X}}(\Phi) \leq v_{f_1,\mathfrak{X}}(\Phi)$ and consequently $v_{f_1,\mathfrak{X}}(\Phi) = v_{f_2,\mathfrak{X}}(\Phi)$.

Next, suppose that $\mathfrak{E}_{f_1,\mathfrak{X}} \subseteq \mathfrak{E}_{f_2,\mathfrak{X}}$. Let id be the identity function on $\mathfrak{R}^m$. Clearly, the Elfving set of the model $(f_i, \mathfrak{X})$ is equal to the Elfving set of the model $(id, \mathfrak{E}_{f_i,\mathfrak{X}})$ for both $i = 1, 2$. Moreover, by the assumption the experimental domain of $(id, \mathfrak{E}_{f_1,\mathfrak{X}})$ is a subset of the experimental domain of $(id, \mathfrak{E}_{f_1,\mathfrak{X}})$, which implies $\mathcal{M}_{id,\mathfrak{E}_{f_1,\mathfrak{X}}} \subseteq \mathcal{M}_{id,\mathfrak{E}_{f_2,\mathfrak{X}}}$. Therefore

$$v_{f_1,\mathfrak{X}}(\Phi) = v_{id,\mathfrak{E}_{f_1,\mathfrak{X}}}(\Phi) \leq v_{id,\mathfrak{E}_{f_2,\mathfrak{X}}}(\Phi) = v_{f_2,\mathfrak{X}}(\Phi)$$

The proof is closed.

■

It turns out that the Elfving sets of a model and its orthogonal submodel have a simple geometric relation as specified in the next proposition.

Proposition 22 *Let $1 \leq k \leq m$, and let $(g, \mathfrak{X})$ be a k-dimensional orthogonal submodel of an m-dimensional model $(f, \mathfrak{X})$, i.e. $g = \mathbf{U}^T f$ for some $\mathbf{U} \in \mathcal{U}_{m,k}$. Consider the orthogonal projector $\mathbf{P} : \mathfrak{R}^m \to \mathfrak{R}^m$, $\mathbf{P} = \mathbf{U}\mathbf{U}^T$, projecting on a k-dimensional linear subspace of $\mathfrak{R}^m$. Then the projection $\mathbf{P}\mathfrak{E}_{f,\mathfrak{X}}$ is an orthogonal rotation of $\mathfrak{E}_{g,\mathfrak{X}}$, if $k = m$, or $\mathbf{P}\mathfrak{E}_{f,\mathfrak{X}}$ is an orthogonal rotation of $\mathfrak{E}_{g,\mathfrak{X}} \times \{0_{m-k}\}$, if $k < m$.*

Proof. Clearly

$$\mathbf{P}\mathfrak{E}_{f,\mathfrak{X}} = \mathbf{U}\,\mathrm{conv}\left\{\mathbf{U}^T f(\mathfrak{X}) \cup -\mathbf{U}^T f(\mathfrak{X})\right\} = \mathbf{U}\mathfrak{E}_{g,\mathfrak{X}}$$

If $k = m$, then the previous equality proves the proposition. If $k < m$, create an orthogonal matrix $\mathbf{V} \in \mathcal{U}_{m,m}$ such that, in the block-matrix notation, $\mathbf{V} = (\mathbf{U}, u_{k+1}, ..., u_m)$ for some orthonormal vectors $u_{k+1}, ..., u_m \in \mathfrak{R}^m$. We obtain $\mathbf{P}\mathfrak{E}_{f,\mathfrak{X}} = \mathbf{V}\left(\mathfrak{E}_{g,\mathfrak{X}} \times \{0_{m-k}\}\right)$.

■

The meaning of Proposition 22 is that the Elfving sets of all k-dimensional orthogonal submodels of an m-dimensional model $(f, \mathfrak{X})$ essentially correspond to all orthogonal projections of $\mathfrak{E}_{f,\mathfrak{X}}$ on k-dimensional linear subspaces. This geometric view can help us to identify the orthogonal submodel of $(f, \mathfrak{X})$ with the "smallest" Elfving set which in turn gives us the best possible upper bounds on the E_k-optimal values given in Theorem 19. We will demonstrate this approach in Sections 8.2 and 9.4.

Using Theorem 19 we can prove that the E_k-optimal value is bounded from above by the square of the k-radius of $\mathfrak{E}_{f,\mathfrak{X}}$, i.e. the square of the minimal radius of a k-dimensional projection of $\mathfrak{E}_{f,\mathfrak{X}}$ (see Section 1.1 for the definition of $r_k(\mathfrak{E}_{f,\mathfrak{X}})$):

Theorem 23 *Let $(f,\mathfrak{X})$ be an m-dimensional model and let $1 \le k \le m$. Then*

$$v_{f,\mathfrak{X}}(k) \le r_k^2(\mathfrak{E}_{f,\mathfrak{X}})$$

with equality if $k = m$ or if $\lambda_k(\mathbf{M}) < \lambda_{k+1}(\mathbf{M})$ for some Φ_{E_k}-optimal information matrix $\mathbf{M}$, i.e. if $k \in \mathfrak{D}_{f,\mathfrak{X}}(\zeta_k^*)$ for some E_k-optimal design ζ_k^*.

Proof. For any projector $\mathbf{P} \in \mathcal{P}_{m,k}$ we have $\operatorname{diam}(\mathbf{P}\mathfrak{E}_{f,\mathfrak{X}}) = 2 \times \max_{x\in\mathfrak{X}} \|\mathbf{P}f(x)\|$, which is a simple consequence of the continuity of norm and the parallelogram law. Moreover, it is easy to show that $\mathbf{P} \in \mathcal{P}_{m,k}$ if and only if $\mathbf{P} = \mathbf{U}\mathbf{U}^T$ for some $\mathbf{U} \in \mathcal{U}_{m,k}$, in which case $\|\mathbf{P}f(x)\| = \left\|\mathbf{U}^T f(x)\right\|$ for all $x \in \mathfrak{X}$. Therefore

$$\begin{aligned} r_k(\mathfrak{E}_{f,\mathfrak{X}}) &= (1/2) \times \min\nolimits_{\mathbf{P}\in\mathcal{P}_{m,k}} \operatorname{diam}(\mathbf{P}\mathfrak{E}_{f,\mathfrak{X}}) = \min\nolimits_{\mathbf{P}\in\mathcal{P}_{m,k}} \max\nolimits_{x\in\mathfrak{X}} \|\mathbf{P}f(x)\| \\ r_k^2(\mathfrak{E}_{f,\mathfrak{X}}) &= \min\nolimits_{\mathbf{P}\in\mathcal{P}_{m,k}} \max\nolimits_{x\in\mathfrak{X}} \|\mathbf{P}f(x)\|^2 = \min\nolimits_{\mathbf{U}\in\mathcal{U}_{m,k}} \max\nolimits_{x\in\mathfrak{X}} \left\|\mathbf{U}^T f(x)\right\|^2 \end{aligned}$$

If $\mathbf{U} \in \mathcal{U}_{m,k}$, then $(\mathbf{U}^T f, \mathfrak{X})$ is a k-dimensional model and for all $\mathbf{M} \in \mathcal{M}_{\mathbf{U}^T f,\mathfrak{X}}$ we know that $\partial\widetilde{\Phi}_{E_k}(\mathbf{M}) = \{\mathbf{I}_k\}$, which follows from Proposition 4. Hence, by Theorem 6 part "(i)$\Leftrightarrow$(ii)", we see that $\max_{x\in\mathfrak{X}} \left\|\mathbf{U}^T f(x)\right\|^2 = v_{\mathbf{U}^T f,\mathfrak{X}}(k)$. Consequently, $r_k^2(\mathfrak{E}_{f,\mathfrak{X}}) = \min_{\mathbf{U}\in\mathcal{U}_{m,k}} v_{\mathbf{U}^T f,\mathfrak{X}}(k)$, and the proof can be completed using Theorem 19. ■

Clearly, the 1-radius of $\mathfrak{E}_{f,\mathfrak{X}}$ is equal to the smallest distance of two parallel hyperplanes bounding $\mathfrak{E}_{f,\mathfrak{X}}$ from opposite sides, which equals the maximal radius of the sphere inscribed to $\mathfrak{E}_{f,\mathfrak{X}}$. This means that we have obtained a generalization of the result in [20] which states that if the minimal eigenvalue of the E-optimal information matrix has multiplicity 1, then the E-optimal value is the squared radius of the sphere inscribed to $\mathfrak{E}_{f,\mathfrak{X}}$.

Using Theorem 23, we can prove a geometric analogue of the equivalence theorem for universal optimality under the class of orthogonally invariant criteria.

Theorem 24 *A design $\xi \in \Xi_{\mathfrak{X}}$ is optimal for $(f,\mathfrak{X})$ with respect to all orthogonally invariant criteria if and only if*

$$\Phi_{E_k}(\mathbf{M}_{f,\mathfrak{X}}(\xi)) = r_k^2(\mathfrak{E}_{f,\mathfrak{X}}) \text{ for all } k \in \mathfrak{D}_{f,\mathfrak{X}}(\xi)$$

Proof. Suppose that $\xi \in \Xi_{\mathfrak{X}}$. If ξ is universally optimal for $(f,\mathfrak{X})$, then for all $k \in \mathfrak{D}_{f,\mathfrak{X}}(\xi)$ we have $\Phi_{E_k}(\mathbf{M}_{f,\mathfrak{X}}(\xi)) = v_{f,\mathfrak{X}}(k) = r_k^2(\mathfrak{E}_{f,\mathfrak{X}})$, where the last equality follows directly from Theorem 23.

Conversely, assume that $\Phi_{E_k}(\mathbf{M}_{f,\mathfrak{X}}(\xi)) = r_k^2(\mathfrak{E}_{f,\mathfrak{X}})$ for some $\xi \in \Xi_{\mathfrak{X}}$ and all $k \in \mathfrak{D}_{f,\mathfrak{X}}(\xi)$. Then $v_{f,\mathfrak{X}}(k) \ge \Phi_{E_k}(\mathbf{M}_{f,\mathfrak{X}}(\xi)) = r_k^2(\mathfrak{E}_{f,\mathfrak{X}}) \ge v_{f,\mathfrak{X}}(k)$ where, again, the last inequality follows from Theorem 23. This means that $\Phi_{E_k}(\mathbf{M}_{f,\mathfrak{X}}(\xi)) = v_{f,\mathfrak{X}}(k)$, i.e. ξ is E_k-optimal for all $k \in \mathfrak{D}_{f,\mathfrak{X}}(\xi)$. Therefore, ξ is universally optimal by Theorem 11.

■

Notice, that Theorem 24 uses only directly geometrically interpretable k-radii of the Elfving set although, in general, they do *not* fully determine the E_k-optimal values.

An obvious disadvantage of claims based on geometry is that we can confidently intuitively manipulate only with objects of dimension at most 3. While some problems in optimal design can be nontrivial even in dimensions 2 and 3 (see e.g. [5]), the problem of universal optimality is usually simple due to Theorem 24. Consider the following example, which is a special case of the model analyzed in Section 7.2.

Example 25 *(Trigonometric model of the first degree on the full circle.) Let $\mathfrak{X} = [0, 2\pi]$ and let $f(x) = (\cos x, \sin x, 1)^T$. The Elfving set of $(f, \mathfrak{X})$ is clearly the cylinder*

$$\mathfrak{E} = \left\{(x, y, z)^T \in \mathfrak{R}^3 : x^2 + y^2 \leq 1, |z| \leq 1\right\}$$

Let ξ be the uniform design on $\{0, 2\pi/3, 4\pi/3\}$. As can be easily calculated, $\mathbf{M}(\xi) = \mathrm{diag}(1/2, 1/2, 1)$. By Theorem 24, to check the universal optimality of ξ we only need to verify that $\Phi_{E_2}(\mathbf{M}(\xi)) = r_2^2(\mathfrak{E})$ and $\Phi_{E_3}(\mathbf{M}(\xi)) = r_3^2(\mathfrak{E})$. Obviously, the form of $\mathbf{M}(\xi)$ implies $\Phi_{E_2}(\mathbf{M}(\xi)) = 1$ and $\Phi_{E_3}(\mathbf{M}(\xi)) = 2$. But $r_2(\mathfrak{E})$ is the minimal radius of the base of a cylinder circumscribed to $\mathfrak{E}$ which is visibly 1, and $r_3(\mathfrak{E})$ is the radius of the sphere circumscribed to $\mathfrak{E}$, which is $\sqrt{2}$. Universal optimality of ξ is proved.

Chapter 6

BOUNDS ON THE E_K-EFFICIENCY AND THE $\mathbb{O}$-MINIMAL EFFICIENCY BASED ON Φ_P-OPTIMAL DESIGNS

6.1 Bounds on the E_k-optimal values based on Φ_p-optimal designs

In this chapter, we will construct bounds on the E_k-optimal values and the $\mathbb{O}$-minimal efficiency which depend only on the eigenvalues of a known Φ_p-optimal information matrix and are very simple to calculate numerically. Moreover, the results obtained have several theoretical implications pertaining to E-optimality, D-optimality and universal optimality, which generalize e.g. results of Kiefer and Galil in [6].

We will briefly outline the main geometric idea that stands behind the results of this section. Suppose that $\mathbf{M}_\Phi$ is a known positive definite Φ-optimal information matrix for some given differentiable criterion $\Phi \in \mathbb{O}$. Then a lemma of Fan (see e.g. [2] 1.2.1. and ex. 13 p. 12) and the subgradient theorem ([19] Section 7.4.) implies

$$\lambda^T(\mathbf{M})\,\lambda_\downarrow(\nabla\Phi(\mathbf{M}_\Phi)) \leq \mathrm{tr}\,(\mathbf{M}\nabla\Phi(\mathbf{M}_\Phi)) \leq \mathrm{tr}\,(\mathbf{M}_\Phi\nabla\Phi(\mathbf{M}_\Phi))$$

for all information matrices $\mathbf{M}$, where $\lambda_\downarrow$ denotes the vector of eigenvalues in a non-increasing order. Consequently, the eigenvalue vector of any information matrix $\mathbf{M}$ belongs to a *known* polyhedral set $\mathfrak{H}$ bounded by the cone $\mathfrak{R}^m_\leq \cap \mathfrak{R}^m_+$ and a halfspace with normal vector $\lambda_\downarrow(\nabla\Phi(\mathbf{M}_\Phi))$. Consider the functions $\varphi_k : \mathfrak{R}^m_+ \to \mathfrak{R}$, where $\varphi_k(z)$ is the sum the k smallest components of z, $k = 1, ..., m$. On $\mathfrak{H}$, the functions φ_k are linear, therefore the E_k-optimal value must be bounded from above by maximum of φ_k on the vertices of $\mathfrak{H}$.

To facilitate manipulations with the vertices of the polyhedral set $\mathfrak{H}$ described above, we will introduce the following notation. Consider a vector $\mu \in \mathfrak{R}^m_{++}$ and define $z_0(\mu) = 0_m$, $z_m(\mu) = \left(\sum_{i=1}^m \mu_i\right)^{-1} 1_m$, and

$$z_s(\mu) = \left(\sum\nolimits_{i=m-s+1}^{m} \mu_i\right)^{-1} \times \left(0^T_{m-s}, 1^T_s\right)^T$$

for $s = 1, ..., m-1$.

Lemma 26 *Let $\mu \in \mathfrak{R}^m_{++}$. Then*

$$\left\{\lambda \in \mathfrak{R}^m_+ \cap \mathfrak{R}^m_\leq : \lambda^T\mu \leq 1\right\} = \mathrm{conv}\left\{z_0(\mu), ..., z_m(\mu)\right\}$$

Proof. Let $\mu \in \mathfrak{R}^m_{++}$, $\lambda \in \mathfrak{R}^m_+ \cap \mathfrak{R}^m_{\leq}$, and $\lambda^T\mu \leq 1$. Set $\alpha_0 = 1 - \lambda^T\mu$, $\alpha_m = \left(\sum_{i=1}^m \mu_i\right)\lambda_1$ and $\alpha_s = \left(\sum_{i=m-s+1}^m \mu_i\right)(\lambda_{m-s+1} - \lambda_{m-s})$ for all $s = 1, ..., m-1$. It is simple to check that $\alpha_s \geq 0$ for all $s = 0, 1, ..., m$, $\sum_{s=0}^m \alpha_s = 1$, and $\sum_{s=0}^m \alpha_s z_s(\mu) = \lambda$. This proves the inclusion "$\subseteq$" in the lemma. The opposite inclusion is clear.

■

Now we can prove the basic theorem of this chapter. Recall that $v(k) = v_{f,\mathfrak{X}}(k)$ denotes the E_k-optimal value of the model $(f, \mathfrak{X})$.

Theorem 27 *([9]) Let $p \in (-\infty, 1]$, let ξ_p^* be a Φ_p-optimal design and let $0 < \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_m$ be all eigenvalues of $\mathbf{M}\left(\xi_p^*\right)$ repeated according to their multiplicities. Then for any $k \in \{1, ..., m\}$:*

$$v(k) \leq \max_{r=1,...,k} \frac{r \times \sum\limits_{i=1}^m \lambda_i^p}{\sum\limits_{i=k+1-r}^m \lambda_i^{p-1}}$$

Proof. Let $p \in (-\infty, 1]$, ξ_p^* be a Φ_p-optimal design, $\mathbf{M}_p = \mathbf{M}\left(\xi_p^*\right)$, and $\lambda = \lambda(\mathbf{M}_p) \in \mathfrak{R}^m_{++}$ and $k \in \{1, ..., m\}$. The function Φ_p is differentiable in $\mathbf{M}_p$ with gradient

$$\nabla\Phi_p(\mathbf{M}_p) = \frac{1}{m}\Phi_p^{1-p}(\mathbf{M}_p)\mathbf{M}_p^{p-1}$$

Let $\mathbf{N}_k$ be any Φ_{E_k}-optimal information matrix. Using a lemma of Fan (see e.g. [2] 1.2.1. and ex. 13 p. 12) and the subgradient theorem ([19] part 7.4.) we obtain

$$\lambda^T(\mathbf{N}_k)\lambda_\downarrow(\nabla\Phi_p(\mathbf{M}_p)) \leq \operatorname{tr}(\mathbf{N}_k\nabla\Phi_p(\mathbf{M}_p)) \leq \operatorname{tr}(\mathbf{M}_p\nabla\Phi_p(\mathbf{M}_p)) = \Phi_p(\mathbf{M}_p)$$

Therefore $\lambda^T(\mathbf{N}_k)\mu \leq 1$ where

$$\mu = \Phi_p^{-1}(\mathbf{M}_p)\lambda_\downarrow(\nabla\Phi_p(\mathbf{M}_p)) = \left(\sum_{i=1}^m \lambda_i^p\right)^{-1} \times \left(\lambda_1^{p-1}, ..., \lambda_m^{p-1}\right)^T \in \mathfrak{R}^m_{++}$$

By Lemma 26 we obtain

$$\lambda(\mathbf{N}_k) \in \operatorname{conv}\{z_0(\mu), ..., z_m(\mu)\}$$

For $\gamma \in \mathfrak{R}^m_+$ let $\varphi_k(\gamma)$ be the sum of the k smallest components of γ. The function φ_k is linear and nonnegative on the convex and compact set $\operatorname{conv}\{z_0(\mu), ..., z_m(\mu)\} \subset \mathfrak{R}^m_+ \cap \mathfrak{R}^m_{\leq}$, which together with $z_0(\mu) = 0_m$ entails that the maximum of φ_k is attained on $z_1(\mu)$, $z_2(\mu)$, ... or $z_m(\mu)$. Therefore

$$\begin{aligned} v(k) = \Phi_{E_k}(\mathbf{N}_k) = \varphi_k(\lambda(\mathbf{N}_k)) \leq \max_{s=1,...,m} \varphi_k(z_s(\mu)) = \\ = \sum_{i=1}^m \lambda_i^p \max_{s=1,...,m} \varphi_k\left(z_s\left(\lambda_1^{p-1}, ..., \lambda_m^{p-1}\right)\right) = \\ = \sum_{i=1}^m \lambda_i^p \max_{r=1,...,k} r \times \left(\sum_{i=k+1-r}^m \lambda_i^{p-1}\right)^{-1} \end{aligned}$$

The proof is complete.

■

Note that once we know the eigenvalues of a regular Φ_p-optimal design, computation of the bounds from Theorem 27 is based on a finite number of elementary arithmetic operations or comparisons and can be readily implemented in any programming language.

6.2 Bounds on the E and T-efficiency based on Φ_p-optimal designs

The formula given in Theorem 27 directly leads to simple bounds on the E-efficiency of Φ_p-optimal designs.

Theorem 28 *([9]) Let $p \in (-\infty, 1]$, let ξ_p^* be a Φ_p-optimal design and let $0 < \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_m$ be all eigenvalues of $\mathbf{M}\left(\xi_p^*\right)$. Then the E-efficiency of ξ_p^* satisfies*

$$\mathrm{eff}\left(\xi_p^* | \Phi_{E_1}\right) \geq \frac{1 + \left(\frac{\lambda_2}{\lambda_1}\right)^{p-1} + ... + \left(\frac{\lambda_m}{\lambda_1}\right)^{p-1}}{1 + \left(\frac{\lambda_2}{\lambda_1}\right)^{p} + ... + \left(\frac{\lambda_m}{\lambda_1}\right)^{p}}$$

Notice, that the formula for the lower bound on the E-efficiency of a D-optimal design is particularly simple:

$$\mathrm{eff}\left(\xi_0^* | \Phi_{E_1}\right) \geq \frac{1}{m} \sum_{i=1}^{m} \frac{\lambda_1}{\lambda_i}$$

It turns out that the bound from Theorem 28 can not drop under a certain fixed positive level independent of the values $\lambda_1, \lambda_2, ..., \lambda_m$. More precisely, consider the following generalization of Theorem 5.1. from [6].

Theorem 29 *([9]) Let $m \geq 1$, $p \in (-\infty, 0]$ and let ξ_p^* be a Φ_p-optimal design. If h is the multiplicity of the minimal eigenvalue of $\mathbf{M}\left(\xi_p^*\right)$ then*

$$\mathrm{eff}\left(\xi_p^* | \Phi_{E_1}\right) \geq \min_{x \in [0,1]} \frac{1 + (m/h - 1)x^{1-p}}{1 + (m/h - 1)x^{-p}}$$

In particular, for a D-optimal design ξ_0^* and for an A-optimal design ξ_{-1}^*:

$$\mathrm{eff}\left(\xi_0^* | \Phi_{E_1}\right) \geq \frac{h}{m} \text{ and } \mathrm{eff}\left(\xi_{-1}^* | \Phi_{E_1}\right) \geq \frac{2}{1 + \sqrt{m/h}}$$

Proof. The claim is simple for $p = 0$. Let $p \in (-\infty, 0)$ and $h, m \in \mathfrak{N}$ be such that $h < m$. Notice that Theorem 28 entails $\mathrm{eff}\left(\xi_p^* | \Phi_{E_1}\right) \geq g(x^*)$, where $x^* \in [0,1]^{m-h}$ is the minimum of the continuous function $g : [0,1]^{m-h} \to (0,1)$ defined by

$$g(x_1, ..., x_{m-h}) = \frac{h + x_1^{1-p} + ... + x_{m-h}^{1-p}}{h + x_1^{-p} + ... + x_{m-h}^{-p}}$$

Firstly, we will show that x^* does not lie at the boundary of the cube $[0,1]^{m-h}$. Suppose that $x_i^* = 0$ or $x_i^* = 1$ for some $i \in \{1, ..., m-h\}$. Choose any positive $\delta < g(x^*)$ and take $x^- \in [0,1]^{m-h}$ such that $x_i^- = \delta$ and $x_j^- = x_j^*$ for $j \neq i$. One can easily verify that then $g(x^-) < g(x^*)$, which contradicts the assumption that x^* minimizes g on $[0,1]^{m-h}$.

Therefore $x^* \in (0,1)^{m-h}$ and since g is smooth on $(0,1)^{m-h}$, x^* must be a stationary point of g. Using elementary calculus we can verify that $\nabla g(x^*) = 0_{m-h}$

implies $x_1^* = ... = x_{m-h}^*$. Consequently $g(x^*) = \min_{x\in[0,1]} g(x, ..., x, x)$ which closes the proof. (The lower bound for A-optimality is a straightforward application of the general formula.)

■

Although for $h = 1$ Theorem 29 gives the same results as the Theorem 5.1. from [6], the difference in favor of Theorem 29 can be considerable in the case of a high multiplicity h of the minimal eigenvalue, as is for instance in the model of spring balance weighing analyzed in Chapter 8.

For a general $p \in (-\infty, 0)$, calculation of the lower bound from Theorem 29 assumes computation of a stationary point of $(1 + (m/h - 1)x^{1-p})\,(1 + (m/h - 1)x^{-p})^{-1}$, i.e. the point $x_0 \in (0, 1)$ which satisfies $q(x_0) = 0$, where

$$q(x) = (m - h)\,x^{1-p} + h(1 - p)x + hp$$

Although x_0 can be explicitly found only for special values $p < 0$ (such as $p = -1$), it is very simple to calculate numerically. One can verify that $q(0) = ph < 0$, $q(1) = m > 0$, next $dq(x)/dx = (1 - p)(h + (m - h)x^{-p}) > 0$ and $d^2q(x)/dx^2 = -px^{-1-p}(m - h)(1 - p) > 0$ for all $x \in (0, 1)$. These properties make finding the root of q a textbook example suitable for an application of the Newton's method with the starting point 1.

Using Theorem 29 for $h = 1$, given $m = 2, ..., 10$, and an efficiency $eff = 0.9, 0.95, 0.99$ we can thus easily find integer values of p, which are enough extreme to guarantee that eff $(\xi_p|\Phi_{E_1}) \geq eff$ (independently of the actual eigenvalues of $\mathbf{M}(\xi_p^*)$).

	m=2	m=3	m=4	m=5	m=6	m=7	m=8	m=9	m=10
eff=0.90	-3	-4	-6	-7	-8	-9	-9	-10	-10
eff=0.95	-5	-9	-12	-14	-16	-18	-19	-20	-21
eff=0.99	-28	-46	-60	-71	-81	-89	-97	-103	-110

For the T-efficiency of Φ_p-optimal designs we obtain:

Theorem 30 *Let $p \in (-\infty, 1]$, let $\xi_p^* \in \Xi$ be Φ_p-optimal, and let $0 < \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_m$ be all eigenvalues of $\mathbf{M}\left(\xi_p^*\right)$. Then the T-efficiency of ξ_p^* satisfies*

$$\text{eff}\left(\xi_p^*|\Phi_{E_m}\right) \geq \frac{\frac{\lambda_1}{\lambda_m} + ... + \frac{\lambda_{m-1}}{\lambda_m} + 1}{\left(\frac{\lambda_1}{\lambda_m}\right)^p + ... + \left(\frac{\lambda_{m-1}}{\lambda_m}\right)^p + 1}$$

Very similarly as for the E-efficiency, it is possible to construct lower bounds on the T-efficiency of a Φ_p-optimal design depending only on m and p or the multiplicity of the largest eigenvalue of the Φ_p-optimal information matrix. However, such bounds would be of limited use, because it is usually easy to construct T-optimal designs directly (unlike E-optimal designs) and find the *exact* value of eff $\left(\xi_p^*|\Phi_{E_m}\right)$.

6.3 The $\mathbb{O}$-minimal efficiency of Φ_p-optimal designs

Based on Theorem 27 and one or more Φ_p-optimal designs, we can construct upper bounds on all unknown E_k-optimal values and consequently lower bounds on the $\mathbb{O}$-minimal efficiency of any given design. Making use of the eigenvalues of the information matrix corresponding to a Φ_p-optimal design ξ_p^*, we can find a lower bound on the $\mathbb{O}$-minimal efficiency of ξ_p^* itself.

Theorem 31 *Let $p \in (-\infty, 1]$, let ξ_p^* be Φ_p-optimal and let $0 < \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_m$ be all eigenvalues of $\mathbf{M}\left(\xi_p^*\right)$. Then*

$$\operatorname{mineff}(\xi_p^*|\mathbb{O}) \geq \min_{1 \leq r \leq k \leq m} \frac{\sum\limits_{i=1}^{k} \lambda_i \times \sum\limits_{i=k-r+1}^{m} \lambda_i^{p-1}}{r \times \sum\limits_{i=1}^{m} \lambda_i^p}$$

The bound from the previous theorem can be easily coded in any programming language with extremely quick numerical computation. The most important theoretical corollary of Theorem 31 is that any D-optimal design has efficiency at least $1/m$ with respect to an arbitrary orthogonally invariant criterion in any model. This is a trivial consequence of the next theorem.

Theorem 32 *Let ξ_0^* be a D-optimal design and let every eigenvalue of the D-optimal information matrix has multiplicity at least h. Then* $\operatorname{mineff}(\xi_0^*|\mathbb{O}) \geq h/m$.

Proof. Let h be the minimal multiplicity of an eigenvalue of $\mathbf{M}(\xi_0^*)$ and let $\lambda = \lambda(\mathbf{M}(\xi_0^*))$. Theorem 32 follows directly from Theorem 31 once we show that

$$\sum_{i=1}^{k} \lambda_i \times \sum_{j=k-r+1}^{m} \lambda_j^{-1} \geq hr \text{ for any } r, k \in \mathfrak{N} \text{ such that } 1 \leq r \leq k \leq m.$$

While the proof of this claim can be based on elementary considerations, the choice of the steps is not completely straightforward, therefore we shall describe it in its full length. We will split the proof into two cases.

Firstly, suppose that $\lambda_{k-r+1} = \lambda_k$. Let $s, t \geq 0$ be the maximal possible whole numbers satisfying $\lambda_{k-r+1-s} = \lambda_{k+t}$. Because the multiplicity of λ_k is at least h, we have $(k+t) - (k-r+1-s) + 1 \geq h$, hence $r + s + t \geq h$. Therefore

$$\begin{aligned} \sum_{i=1}^{k} \lambda_i \times \sum_{j=k-r+1}^{m} \lambda_j^{-1} \geq \sum_{i=k-r+1-s}^{k} \lambda_i \times \sum_{j=k-r+1}^{k+t} \lambda_j^{-1} = \\ = \{k - (k-r+1-s) + 1\} \times \{(k+t) - (k-r+1) + 1\} = \\ = (r+s)(r+t) = r(r+s+t) + st \geq rh + st \geq rh \end{aligned}$$

Secondly, suppose that $\lambda_{k-r+1} < \lambda_k$. Let s, t be the maximal possible whole numbers and let z be the (only one) whole number such that $\lambda_{k-r+1-s} = \lambda_{k-r+1} = \lambda_{k-z} < \lambda_{k-z+1} = \lambda_{k+t}$. (Note that $s \geq 0$, but t can be negative.) Clearly $z \geq 1$ and $r \geq z + 1$, which means that $z(r-z) \geq 0$. The multiplicity of λ_{k-r+1} is at least h, which implies $(k-z) - (k-r+1-s) + 1 \geq h$, therefore $r + s - z \geq h$. Similarly, because the multiplicity of λ_{k-z+1} is at least h we obtain $(k+t) - (k-z+1) + 1 \geq h$, which means $t + z \geq h$. Using these inequalities we get

$$\sum_{i=1}^{k} \lambda_i \times \sum_{j=k-r+1}^{m} \lambda_j^{-1} \geq \sum_{i=k-r+1-s}^{k-z} \lambda_i \times \sum_{j=k-r+1}^{k-z} \lambda_j^{-1} + \sum_{i=k-z+1}^{k} \lambda_i \times \sum_{j=k-r+1}^{k+t} \lambda_j^{-1} \geq$$
$$\geq \{(k-z)-(k-r+1-s)+1\} \times \{(k-z)-(k-r+1)+1\} +$$
$$+ \{k-(k-z+1)+1\} \times \{(k+t)-(k-r+1)+1\} =$$
$$= (r+s-z)(r-z) + z(r+t) \geq h(r-z) + z(r-z) + z(z+t) \geq h(r-z) + zh = hr$$

■

Interestingly, for the designs which are optimal with respect to other Kiefer's criteria (not Φ_0), there does not exist a similar general lower bound as $1/m$. (This follows e.g. from Theorem 5.2 in [6].) In other words, for $p \neq 0$ any positive lower bound on the $\mathbb{O}$-minimal efficiency of a Φ_p-optimal design must take some properties of the model into account (e.g. we must know the eigenvalues of the Φ_p-optimal information matrix, which *do* depend on f and $\mathfrak{X}$). Moreover, the bound $1/m$ on the $\mathbb{O}$-minimal efficiency of the D-optimal design is largest possible in the sense that there exist m-dimensional models, such that $\text{mineff}(\xi_0^*|\mathbb{O})$ is arbitrarily close to $1/m$ (see the last paragraph in the Section 9.5).

Although behavior of the bound from Theorem 31 as a function of λ seems to be complicated for general m and p, it can be substantially simplified for small values of m and/or special criteria Φ_p. The proofs of the next two propositions are mechanical and omitted.

Theorem 33 *Let $m = 2$, $p \in (-\infty, 1]$, let ξ_p^* be a Φ_p-optimal design and let $0 < \lambda_1 \leq \lambda_2$ be the eigenvalues of $\mathbf{M}\left(\xi_p^*\right)$. Then*

$$\text{mineff}(\xi_p^*|\mathbb{O}) \geq \begin{cases} \left(1 + \frac{\lambda_1}{\lambda_2}\right) : \left(1 + \left(\frac{\lambda_1}{\lambda_2}\right)^p\right) & \text{if } p \leq 0 \\ \left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^{p-1}\right) : \left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^p\right) & \text{if } p \geq 0 \end{cases}$$

If $\lambda_1 = 0$ then $\text{mineff}(\xi_p^*|\mathbb{O}) = 0$.

For $p = 0$ (D-optimal design) and for $p = -1$ (A-optimal design), the bound from Theorem 33 is

$$\text{mineff}(\xi_0^*|\mathbb{O}) \geq \frac{1}{2}\left(1 + \frac{\lambda_1}{\lambda_2}\right) \text{ and } \text{mineff}(\xi_{-1}^*|\mathbb{O}) \geq \frac{\lambda_1}{\lambda_2}$$

For the case $m = 3$ the bounds for D and A-optimal designs are given in the next theorem.

Theorem 34 *Let $m = 3$, and let ξ_0^*, ξ_{-1}^* be the D- and the A-optimal designs. Denote by $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3$ the eigenvalues of $\mathbf{M}(\xi_0^*)$, resp. $\mathbf{M}\left(\xi_{-1}^*\right)$. Then*

$$\text{mineff}(\xi_0^*|\mathbb{O}) \geq \frac{1}{3}\min\left\{1 + \frac{\lambda_1}{\lambda_2} + \frac{\lambda_1}{\lambda_3}, 1 + \frac{\lambda_2}{\lambda_3} + \frac{\lambda_1}{\lambda_3}\right\}$$

$$\text{mineff}(\xi_{-1}^*|\mathbb{O}) \geq \frac{(\lambda_1 + \lambda_2 + \lambda_3)\,\lambda_3^{-2}}{\lambda_1^{-1} + \lambda_2^{-1} + \lambda_3^{-1}}$$

Obviously, the bounds from Theorem 34 depend only on the ratios of components of λ, which means that they can be visualized as real functions defined on the simplex $\left\{(\lambda_1, \lambda_2, \lambda_3)^T \in \mathfrak{R}_+^3 : \sum_{i=1}^3 \lambda_i = 1\right\}$. For this case the contour plots of the lower bounds are exhibited in the Figures 1 and 2 in the Appendix.

6.4 Universal optimality of Φ_p-optimal designs

At the end of this chapter, we will prove two sufficient conditions on universal optimality of designs under the class of orthogonally invariant criteria.

Theorem 35 *([9]) If a design ξ_p^* is Φ_p-optimal for some $p \in (-\infty, 1]$ and if $\mathbf{M}(\xi_p^*)$ is a positive multiple of the identity matrix, then ξ_p^* is optimal with respect to all orthogonally invariant criteria.*

Proof. Let $p \in (-\infty, 1]$ and for the Φ_p-optimal design ξ_p^* let $\mathbf{M}\left(\xi_p^*\right) = \delta \mathbf{I}_m$, $\delta > 0$. Direct application of Theorem 27 implies that the Φ_{E_m}-optimal value is $v(m) \leq \delta m$. This clearly entails E_m-optimality of ξ_p^*, because $\Phi_{E_m}(\mathbf{M}\left(\xi_p^*\right)) = \delta m$. By Theorem 12, ξ_p^* is optimal with respect to all $\Phi \in \mathbb{O}$.

■

We remark that Theorem 35 can not be extended to cover the case of E-optimality ($p = -\infty$). For example in the model of spring balance weighing of degree $m = 2$, the E-optimal information matrix is a scalar multiple of the identity matrix, yet it is *not* optimal for all $\Phi \in \mathbb{O}$ (e.g. it is not D-optimal; see Theorem 46 in Chapter 8).

Theorem 36 *([9]) If a design ξ^* is Φ_p-optimal for all $p \in (-\infty, 1)$ and if $\mathbf{M}(\xi^*)$ has at most two distinct eigenvalues, then ξ^* is optimal with respect to all orthogonally invariant criteria.*

Proof. Let ξ^* be Φ_p-optimal for all $p \in (-\infty, 1)$ and let $\mathbf{M}(\xi^*)$ have at most two distinct eigenvalues. If all the eigenvalues of $\mathbf{M}(\xi^*)$ are the same then Theorem 36 follows from Theorem 35. Therefore we can assume that $\lambda(\mathbf{M}(\xi^*)) = (\lambda, ..., \lambda, \gamma, ..., \gamma)^T$, $\lambda < \gamma$ and the multiplicity of λ is $s \leq m - 1$.

Denote by $u_k(p)$ the upper bound on $v(k)$ given by Theorem 27 taken in $p \in (-\infty, 1)$. By the assumption of Theorem 36 we have $v(k) \leq \inf_{p \in (-\infty,1)} u_k(p)$. But it can be verified that:

1) For $k \in \{1, ..., s\}$: $\lim_{p \to -\infty} u_k(p) = k\lambda$;
2) For $k \in \{s+1, ..., m-1\}$: $u_k(1 - \log_{\gamma/\lambda} \frac{m-s}{k-s}) = s\lambda + (k-s)\gamma$;
3) $\lim_{p \to 1} u_m(p) = s\lambda + (m-s)\gamma$.

Consequently $\inf_{p \in (-\infty,1)} u_k(p) = \Phi_{E_k}(\mathbf{M}(\xi^*))$ i.e. ξ^* is E_k-optimal for all $k = 1, ..., m$. Using Theorem 10 this implies optimality of ξ^* with respect to all orthogonally invariant criteria.

■

The previous theorem can be used to prove universal optimality for the equidistant support design in trigonometric regression (see Theorem 40 in Chapter 7). We also remark that for the model of spring balance weighing (Chapter 8) it can be shown that for an odd degree $m > 1$ the D-optimal design ξ_0^* is Φ_p-optimal for all $p \in [-\infty, 0]$, the information matrix $\mathbf{M}(\xi_0^*)$ has only two distinct eigenvalues, yet ξ_0^* is not optimal with respect to all orthogonally invariant criteria (e.g. ξ_0^* is not T-optimal). In combination with Theorem 36 this fact means that Φ_p-optimality for all the most studied $p \in [-\infty, 0]$ is generally much weaker than Φ_p-optimality for the complete class including also the less popular positive values of p.

Part III

ANALYSIS OF SPECIFIC MODELS

Chapter 7

MODELS ADMITTING A UNIVERSALLY OPTIMAL DESIGN

7.1 Universal optimality in regression on a sphere

In this chapter, we will analyse several of the most important models admitting a design optimal with respect to all orthogonally invariant criteria. We begin with the model on the Euclidean m-dimensional sphere.

Consider the model $(f, \mathfrak{X})$, where $f(x) = x$ and $\mathfrak{X} = \{x \in \mathfrak{R}^m : \sum_{i=1}^m x_i^2 = r^2\}$ is the m-dimensional sphere with origin in $0_m = (0, ..., 0) \in \mathfrak{R}^m$ and diameter $r > 0$.

Theorem 37 *A design $\xi \in \Xi$ is optimal for the model $(f, \mathfrak{X})$ with respect to all orthogonally invariant criteria if and only if $\mathbf{M}(\xi) = \frac{r^2}{m}\mathbf{I}_m$.*

Proof. If $\mathbf{M}(\xi) = \frac{r^2}{m}\mathbf{I}_m$, then ξ is T-optimal, because it satisfies conditions given by the equivalence theorem 6: $\mathrm{tr}(\mathbf{M}(\xi)) = r^2 = \max_{x\in\mathfrak{X}} \|x\|^2$. By Theorem 11, ξ is then optimal with respect to all $\Phi \in \mathbb{O}$.

Conversely, let ξ be universally optimal for $(f, \mathfrak{X})$. Notice, that the design $\xi^{/}$ uniform on $\{r \times e_i, i = 1, ..., m\}$, where e_i are the basic unit vectors in $\mathfrak{R}^m$, has information matrix $\frac{r^2}{m}\mathbf{I}_m$, i.e. $\xi^{/}$ is universally optimal by the first proved part of the theorem. Since ξ is E-optimal, we have $\lambda_1(\mathbf{M}(\xi)) \geq \lambda_1(\mathbf{M}(\xi^{/})) = \frac{r^2}{m}$ and since $\xi^{/}$ is T-optimal, we have $\mathrm{tr}(\mathbf{M}(\xi)) \leq \mathrm{tr}(\mathbf{M}(\xi^{/})) = r^2$. Consequently, all the eigenvalues of $\mathbf{M}(\xi)$ are equal to $\frac{r^2}{m}$ which entails $\mathbf{M}(\xi) = \frac{r^2}{m}\mathbf{I}_m$.

■

Obviously, there is a multitude of designs with information matrix $\frac{r^2}{m}\mathbf{I}_m$, being thus universally optimal for $(f, \mathfrak{X})$. (An exception is the trivial case $m = 1$ with only one such design.) In fact, any uniform design on $\mathfrak{X}$ invariant under a sufficiently rich group of rotations is also universally optimal:

Proposition 38 *Let $\mathcal{G} \subseteq \mathcal{U}_{m,m}$ be a group of orthogonal matrices such that*

$$\mathrm{span}\{\mathbf{U}v : \mathbf{U} \in \mathcal{G}\} = \mathfrak{R}^m \textit{ for all } v \in \mathfrak{R}^m$$

Let $\mathfrak{G} \subseteq \mathfrak{X}$ be a finite set invariant under all members of $\mathcal{G}$. Then any design $\xi \in \Xi$ uniform on $\mathfrak{G}$ is optimal for $(f, \mathfrak{X})$ with respect to all orthogonally invariant criteria.

Proof. Let ξ satisfy the assumptions of the theorem. Let u be any eigenvector of $\mathbf{M} = \mathbf{M}(\xi)$ with a positive eigenvalue λ (there is such a vector since $\mathbf{M}$ is not the zero matrix). Let $\mathbf{U} \in \mathcal{G}$. Because the support of ξ is invariant under $\mathbf{U}$, we have $\mathbf{M} = \mathbf{UMU}^T$. Hence, $\mathbf{M}u=\lambda u$ implies $\mathbf{UMU}^T u = \lambda u = \lambda \mathbf{UU}^T u$, therefore $\mathbf{M}\left(\mathbf{U}^T u\right) = \lambda \left(\mathbf{U}^T u\right)$. This means that $\mathbf{U}^T u$ is also an eigenvector of $\mathbf{M}$ with eigenvalue λ, and as $\mathbf{U}$ was an arbitrary member of $\mathcal{G}$ we see that all the vectors in $\{\mathbf{U}v : \mathbf{U} \in \mathcal{G}\}$ are eigenvectors with the same eigenvalue λ. From the assumption we conclude that the entire $\mathfrak{R}^m$ is an eigenspace corresponding to λ which implies $\mathbf{M} = \lambda \mathbf{I}_m$. Moreover, as $x^T x = r^2$ for all $x \in \mathfrak{X}$:

$$m\lambda = \mathrm{tr}(\lambda \mathbf{I}_m) = \mathrm{tr}(\mathbf{M}) = \mathrm{tr}\left(\sum_{x\in\mathfrak{X};\xi(x)>0} \xi(x) x^T x\right) = r^2$$

We obtained $\lambda = r^2/m$, which completes the proof in view of Theorem 37.

■

Any group of rotations satisfying the condition from Theorem 38 yields universally optimal designs as uniform probabilities on orbits of finite sets. Naturally, we can form convex combinations of such designs to create another universally optimal designs. Thus, while the universally optimal informtion matrix is unique and simple, the set of all universally optimal designs has a very complex structure.

Using Theorem 11 we can also easily solve the problem of universal optimality for the general model on the l_p-sphere. Let $f(x) = x$ for $x \in \mathfrak{R}^m$ and $\mathfrak{X}(p,r) = \left\{x \in \mathfrak{R}^m : \|x\|_p = r\right\}$, where $r > 0$ and the l_p-norm of x is defined by $\|x\|_p = \left(\sum_{i=1}^m |x_i|^p\right)^{1/p}$ for $1 \le p < \infty$ and $\|x\|_\infty = \max\{|x_1|, ..., |x_m|\}$. For $p = -\infty$ this model is known under the name "chemical balance weighing".

Theorem 39 *If $1 \le p \le 2$, let ξ be the uniform design on $\{r \times e_1, ..., r \times e_m\}$, where $e_i \in \mathfrak{R}^m$ are the basic unit vectors. If $2 \le p \le \infty$, let ξ be the uniform design on the 2^m vectors of the form $rm^{-1/p} \times (\pm 1, ..., \pm 1)^T \in \mathfrak{R}^m$. Then ξ is optimal for the model $(f, \mathfrak{X}(p,r))$ with respect to all orthogonally invariant criteria.*

Proof. If $1 \le p \le 2$, then $\mathbf{M}(\xi) = \frac{r^2}{m}\mathbf{I}_m$ and if $2 \le p \le \infty$ then $\mathbf{M}(\xi) = \frac{r^2}{m^{2/p}}\mathbf{I}_m$, which can be directly verified. By Theorem 12, we only need to check that ξ is T-optimal, i.e. that $\mathrm{tr}(\mathbf{M}(\xi))$ is the maximum of the (Euclidean) norm of $\|x\|^2$ over $\mathfrak{X}(p,r)$. But this is a simple consequence of the inequality $\|\cdot\|_p \ge \|\cdot\|_2$ valid for $1 \le p \le 2$ and the inequality $\|\cdot\|_p \ge m^{2/p-1}\|\cdot\|_2$ valid for $2 \le p \le \infty$ (cf. [4], Example 4.2.).

■

The authors of the article [4] prove E-optimality of the designs from the previous theorem using spheres inscribed to a generalized Elfving set consisting of matrices. Application of this intriguing yet difficult technique is in contrast with the mechanical proof based on Theorem 11.

7.2 Universal optimality in trigonometric regression

Consider the trigonometric regression model of the degree d on the full circle, i.e. the model $(f, \mathfrak{X})$, where

$$f(x) = (\cos x, \sin x, \cos 2x, \sin 2x, ..., \cos dx, \sin dx, 1)^T$$

and $\mathfrak{X} = [0, 2\pi]$, with $m = 2d + 1$ parameters.

It has already been shown that the design ξ^* which is uniform on

$$\{2k\pi/m + \pi : k = -d, -d+1, ..., d-1, d\}$$

is Φ_p-optimal for any $p \in [-\infty, 1]$ (see e.g. [19], Section 9.16.) and also Φ_{Ch_k}-optimal for any $k = 1, ..., m$ (see [25]). We will prove the following generalization of these results.

Theorem 40 *([8], [9]) Design ξ^* is optimal for $(f, \mathfrak{X})$ with respect to all orthogonally invariant criteria.*

Proof. Similarly as in the proof of Proposition VI.9 in [17] or Claim 9.16. in [19], we can show that $\mathbf{M}^* = \mathbf{M}(\xi^*) = \mathrm{diag}(1/2, ..., 1/2, 1)$. As ξ^* is Φ_p-optimal for all $p \in [-\infty, 1]$, and $\mathbf{M}^*$ has only two distinct eigenvalues, Theorem 40 immediately follows from Theorem 36. For the sake of demonstration of compatibility of results given in this work, we will also show a second, completely different proof based on results of Section 4.2.

Using Theorem 12 and the fact that ξ^* is T-optimal, we see that we only need to check that ξ^* is E_{m-1}-optimal. This requires verifying that $\max_{x\in\mathfrak{X}} \left\|\mathbf{U}^T f(x)\right\|^2 = \Phi_{E_{m-1}}(\mathbf{M}^*)$, where $\mathbf{U}$ is *any* matrix with columns being an orthonormal basis of the $m-1$ dimensional eigenspace corresponding to the eigenvalue $1/2$ of $\mathbf{M}^*$. Trivially, $\mathbf{U} = (e_1, ..., e_{m-1})$, where e_i are the basic unit vectors, is such a matrix and for all $x \in \mathfrak{X}$:

$$\left\|\mathbf{U}^T f(x)\right\|^2 = \sum_{j=1}^{\frac{m-1}{2}} \left(\cos^2(jx) + \sin^2(jx)\right) = \frac{m-1}{2} = \Phi_{E_{m-1}}(\mathbf{M}^*)$$

The proof is complete.

■

We remark that the design ξ^* from the previous theorem is not the only universally optimal design for $(f, \mathfrak{X})$. For example it is simple to show that any design which is a convex combination of designs equidistantly spaced on at least $2d+1$ points in $\mathfrak{X}$ is also universally optimal for $(f, \mathfrak{X})$.

7.3 Linear transformation leading to universal optimality

For majority of commonly used models, no design is simultaneously optimal with respect to all orthogonally invariant criteria. (We will analyze several of such models in the subsequent chapters.) Despite of that a simple, but noteworthy fact is that for *any* model there exists a linear reparametrization which does admit a universally optimal design. Such a reparametrization can be directly constructed from the D-optimal information matrix as specified in the following theorem.

Theorem 41 *Let ξ_0^* be a D-optimal design for an m-dimensional model $(f, \mathfrak{X})$. Let $\mathbf{M}(\xi_0^*) = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$ for some orthogonal matrix $\mathbf{U} \in \mathcal{U}_{m,m}$ and a diagonal matrix $\mathbf{\Lambda}$. Let*

$\mathbf{V} \in \mathcal{U}_{m,m}$ be any orthogonal matrix and let $c > 0$. Consider the linear reparametrization $(g, \mathfrak{X})$ of the model $(f, \mathfrak{X})$ given by $g = c\mathbf{V}\mathbf{\Lambda}^{-1/2}\mathbf{U}^T f$. Then ξ_0^* is universally optimal for $(g, \mathfrak{X})$.

Proof. Let ξ_0^* be a D-optimal design for $(f, \mathfrak{X})$. Consider a model $(g, \mathfrak{X})$ as given in the theorem. As D-optimality of a design is preserved by any regular linear reparametrization of the model, we see that ξ_0^* is D-optimal also for $(g, \mathfrak{X})$. But

$$\mathbf{M}_{g,\mathfrak{X}}(\xi_0^*) = c^2\mathbf{V}\mathbf{\Lambda}^{-1/2}\mathbf{U}^T\mathbf{M}_{f,\mathfrak{X}}(\xi_0^*)\left(\mathbf{V}\mathbf{\Lambda}^{-1/2}\mathbf{U}^T\right)^T = c^2\mathbf{I}_m$$

Theorem 41 now follows directly from Theorem 35.

■

For all linear reparametrizations $(\mathbf{A}f, \mathfrak{X})$ of $(f, \mathfrak{X})$, where $\mathbf{A}$ is an arbitrary regular matrix of type $m \times m$, the procedure given by the previous theorem leads to models which are same up to a positive multiple or an orthogonal reparametrization. It can be shown that the transformations given in Theorem 41 correspond to linear deformations of the minimal volume ellipsoid containing the Elfving set of $(f, \mathfrak{X})$ to a sphere.

Apart from being geometrically pleasing, the models constructed using Theorem 41 are usually artificial, without an interpretation of parameters and appeal to a practitioner. In the sequel, we will briefly describe two examples.

Example 42 *(2-way multivariate linear regression of the first degree on $\{0,1\}^2$.) Consider the model $(f, \mathfrak{X})$, where $f(x) = x$ and $\mathfrak{X} = \{0,1\}^2$. It is easy to check that the D-optimal design ξ_0^* is uniform on $\{(1,0), (0,1), (1,1)\}$. A transformation from Theorem 41 based on $\mathbf{M}(\xi_0^*)$ leads to the model $(g, \mathfrak{X})$, where*

$$g(x_1, x_2) = ((x_1 + x_2)/2, \sqrt{3}(x_1 - x_2)/2)^T$$

with ξ_0^* being a universally optimal design. Notice, that the Elfving set of $(g, \mathfrak{X})$ is a regular hexagon inscribed into the unit circle. (See Chapter 8 for these models of a general degree in the standard parametrization.)

Example 43 *(Quadratic polynomial model on $[-1,1]$.) Our initial model is $(f, \mathfrak{X})$, where $f(x) = (1, x, x^2)^T$ and $\mathfrak{X} = [-1,1]$. Using the D-optimal design (the uniform probability on $\{-1,0,1\}$) and Theorem 41 we can construct the model $(g, \mathfrak{X})$, with*

$$g(x) = (\sqrt{2}, \sqrt{3}x,\ -2 + 3x^2)^T$$

admitting a universally optimal design. In this case, the Elfving set of $(g, \mathfrak{X})$ is a convex body touching the circumscribed sphere at vertices of a regular octahedron. (See Chapter 10 for an analysis of the polynomial regression in the standard parametrization.)

Chapter 8

MULTIVARIATE LINEAR REGRESSION OF THE FIRST DEGREE WITHOUT A CONSTANT TERM

8.1 Definition of the model and neighbor-vertex designs

Consider the m-way multivariate linear regression model of the first degree over the unit cube without an intercept term given by the formula:

$$y = x_1\beta_1 + ... + x_m\beta_m + \varepsilon,\ x_1, ..., x_m \in \{0, 1\}$$

For a choice of points $x_1, ..., x_m \in \{0, 1\}$, the value $x_i = 1$ can be interpreted as a presence and $x_i = 0$ as an absence of the i-th item in the balance measuring weight by the tension of a spring. In accord with this interpretation, this model is sometimes called the model of spring balance weighing.

For the model in consideration, the vector of regression functions is $f : \mathfrak{X} \to \mathfrak{R}^m$, $f(x) = x$ and the experimental domain is $\mathfrak{X} = \{0, 1\}^m$. Notice that in the asymptotic design theory, the experimental domain $\mathfrak{X}$ is essentially same as $[0, 1]^m$, because any point from $[0, 1]^m$ can be expressed as a convex combination of points from $\mathfrak{X}$ and, trivially, vice versa.

To the optimal design theory of this model (see e.g. [3] for Φ_p-optimal designs, [4] for a geometric construction of E-optimal designs, or [19] Section 14.10. for a general analysis) we will add results concerning minimal efficiency under the class of orthogonally invariant criteria.

Let $j \in \{0, 1, ..., m\}$ and let κ_j be the j-vertex design, i.e. the uniform probability on the unit cube vertices from $\mathfrak{X}$ having exactly j-components equal to 1 and $m - j$ components equal to 0. Let us extend the set of j-vertex designs to the set of so called neighbor-vertex designs κ_s, such that for a noninteger $s \in [0, m]$ we define

$$\kappa_s = (1 - (s - \lfloor s \rfloor))\kappa_{\lfloor s \rfloor} + (s - \lfloor s \rfloor)\kappa_{\lfloor s \rfloor + 1}$$

In the previous formula, $\lfloor s \rfloor$ denotes the largest integer number not exceeding s. The following proposition is a trivial consequence of the Claim I in [19], p. 374, and explains the importance of the neighbor-vertex designs.

Proposition 44 *Let Φ be an orthogonally invariant criterion. Then there exists $s \in [0, m]$, such that the neighbor-vertex design κ_s is Φ-optimal for the model $(f, \mathfrak{X})$.*

Together with Proposition 44, the next proposition entails that, in principle, construction of a Φ-optimal design can be based on one dimensional calculus.

Proposition 45 *Let $s \in [0, m]$, $m > 1$, and let κ_s be a neighbor-vertex design. Then*

$$\mathbf{M}(\kappa_s) = a_s^{(m)} \left(\mathbf{I}_m - \frac{1}{m} 1_m 1_m^T \right) + b_s^{(m)} \left(\frac{1}{m} 1_m 1_m^T \right)$$

where

$$a_s^{(m)} = \frac{-2s \lfloor s \rfloor - s + \lfloor s \rfloor + \lfloor s \rfloor^2 + sm}{m(m-1)},\ b_s^{(m)} = \frac{2s \lfloor s \rfloor + s - \lfloor s \rfloor - \lfloor s \rfloor^2}{m}$$

Moreover

$$\lambda \left(\mathbf{M}(\kappa_s) \right) = (a_s^{(m)}, ..., a_s^{(m)}, b_s^{(m)})^T$$

Proof. The proposition is a direct consequence of the results in [19] Section 14.10. ■

Propositions 44 and 45 can be used to derive Φ_p-optimal designs for all $p \in [-\infty, 1]$. The E- and D-optimal designs are given in the next proposition.

Proposition 46 *Let $m > 1$. Let $s_{-\infty} = \frac{m}{2}$ and $s_0 = \frac{m}{2} \frac{m+2}{m+1}$ if m is even and let $s_{-\infty} = s_0 = \frac{m+1}{2}$ if m is odd. Then the neighbor-vertex design $\xi_{-\infty}^* = \kappa_{s_{-\infty}}$ is E-optimal and the neighbor-vertex design $\xi_0^* = \kappa_{s_0}$ is D-optimal for the model $(f, \mathfrak{X})$. If m is even then*

$$\lambda \left(\mathbf{M}(\xi_{-\infty}^*) \right) = \left(\frac{1}{4} \frac{m}{m-1}, ..., \frac{1}{4} \frac{m}{m-1}, \frac{m}{4} \right)^T \quad \textit{and}$$

$$\lambda \left(\mathbf{M}(\xi_0^*) \right) = \left(\frac{1}{4} \frac{m+2}{m+1}, ..., \frac{1}{4} \frac{m+2}{m+1}, \frac{m+2}{4} \right)^T$$

and if m is odd then

$$\lambda \left(\mathbf{M}(\xi_{-\infty}^*) \right) = \lambda \left(\mathbf{M}(\xi_0^*) \right) = \left(\frac{1}{4} \frac{m+1}{m}, ..., \frac{1}{4} \frac{m+1}{m}, \frac{1}{4} \frac{(m+1)^2}{m} \right)^T$$

We remark that for an odd $m > 1$, the E-optimal information matrix is *not* unique, which is known to be theoretically possible (because $\Phi_{-\infty}$ is not strictly concave), but rare in non-artificial models. Indeed, if $s_{-\infty}^{/} = \frac{m-1}{2}$ then the information matrix of $\xi_{-\infty}^{/} = \kappa_{s_{-\infty}^{/}}$ has the same minimal eigenvalue as the information matrix of the E-optimal design $\xi_{-\infty}^*$ given in Proposition 46, yet the information matrices themselves differ.

8.2 The E_k-optimal values

For calculation of the $\mathbb{O}$-minimal efficiency of designs and construction of the $\mathbb{O}$-maximin efficient design for $(f, \mathfrak{X})$ we need to find the E_k-optimal values.

Theorem 47 *Let $m > 1$. The E_k-optimal values $v(k)$ for the model $(f, \mathfrak{X})$ are $v(m) = m$ and for all $1 \leq k < m$:*

$$v(k) = \frac{k}{4} \frac{m}{m-1} \textit{ if } m \textit{ is even}, \quad v(k) = \frac{k}{4} \frac{m+1}{m} \textit{ if } m \textit{ is odd}$$

Proof. A technical proof of the theorem can be based on Propositions 44 and 45. Nevertheless, we opt for the use of ideas from Chapter 5. This approach gives us an independent proof of E-optimality of the design from Proposition 46, as well as more insight into the geometry of E_k-optimality in this model.

Evidently, the Elfving set $\mathfrak{E}_{f,\mathfrak{X}}$ of $(f, \mathfrak{X})$ is the convex hull of the union of the cubes $[0,1]^m$ and $[-1,0]^m$. Intutivelly, the "smallest" $m-1$ dimensional projection of $\mathfrak{E}_{f,\mathfrak{X}}$ is orthogonal to the common diagonal of the two cubes, i.e. it is orthogonal to 1_m. Therefore, we will consider the projection

$$\mathbf{P} = \mathbf{U}\mathbf{U}^T = \mathbf{I}_m - \tfrac{1}{m}1_m1_m^T, \text{ where } \mathbf{U} \in \mathcal{U}_{m,m-1},$$

and the $m-1$ dimensional submodel $(g, \mathfrak{X})$ of $(f, \mathfrak{X})$ given by $g = \mathbf{U}^T f$.

We will prove the theorem for an even m, remarking that the case of an odd m is completely analogous. For any unit cube vertex $x \in \mathfrak{X}$ we have

$$\|g(x)\|^2 = x^T \left(\mathbf{I}_m - \tfrac{1}{m}1_m1_m^T\right) x = m\,(\overline{x} - \overline{x}^2),$$

where $\overline{x} = \frac{1}{m}\sum_{i=1}^m x_i$. Hence, the norm $\|g(x)\|$ is maximized at those points $x \in \mathfrak{X}$ such that $\overline{x} = 1/2$, that is at the points with $m/2$ entries equal to 1. The corresponding maximum of $\|g(x)\|$ is thus $\sqrt{m}/2$, which means that the Elfving set $\mathfrak{E}_{g,\mathfrak{X}}$ of $(g, \mathfrak{X})$ is a subset of the ball with radius $r = \sqrt{m}/2$ centered in 0_{m-1}. Therefore, Proposition 21 and Theorem 37 imply that for $1 \leq k \leq m-1$, the E_k-optimal value $v_{g,\mathfrak{X}}(k)$ of the $m-1$ dimensional model $(g, \mathfrak{X})$ can not be larger than $kr^2/(m-1)$. Consequently, for the design $\xi^*_{-\infty}$ given in Proposition 46 we obtain

$$\Phi_{E_k}(\mathbf{M}_{f,\mathfrak{X}}(\xi^*_{-\infty})) = \tfrac{k}{4}\tfrac{m}{m-1} = \tfrac{kr^2}{m-1} \geq v_{g,\mathfrak{X}}(k)$$

By Proposition 17, the previous inequality implies that $\xi^*_{-\infty}$ is E_k-optimal for all $k = 1, ..., m-1$. Hence, the E_k-optimal value of $(f, \mathfrak{X})$ is $\frac{km}{4(m-1)}$.
■

Note, that the previous proof gives us a clear geometric interpretation of the E-optimal values of the model $(f, \mathfrak{X})$: Construct the orthogonal projection of the unit cube $[0,1]^m$ in the direction of its main diagonal. Find the minimal hypersphere $\mathfrak{S}$ circumscribed to this projection. The E-optimal value for the model $(f, \mathfrak{X})$ is then equal to the squared radius of $\mathfrak{S}$ divided by $m-1$.

This is a geometric interpretation alternative to the one given in the paper [4], where the E-optimal values are based on the radius of a sphere inscribed to the extended Elfving set of $m \times m$ dimensional matrices.

For the first 5 dimensions, the following table exhibits the E_k-optimal values.

	m=1	m=2	m=3	m=4	m=5
k=1	1	1/2	1/3	1/3	3/10
k=2	-	2	2/3	2/3	3/5
k=3	-	-	3	1	9/10
k=4	-	-	-	4	6/5
k=5	-	-	-	-	5

8.3 The $\mathbb{O}$-minimal efficiency of the neighbor-vertex designs and the $\mathbb{O}$-maximin efficient designs

Consider the model $(f, \mathfrak{X})$, where $m > 1$. Theorem 47 implies that if $1 \leq k < m$ then the E_k-efficiency of any design ξ is at least as high as the E-efficiency of ξ. Therefore, the $\mathbb{O}$-minimal efficiency of ξ is simply the minimum of the E-efficiency and the T-efficiency of ξ as follows from Theorem 10. Moreover, the design κ_m is T-optimal and $\mathrm{tr}(\mathbf{M}(\kappa_s)) = s$ for all $s \in [0, m]$. We obtain:

Theorem 48 *Let $m > 1$, $s \in [0, m]$, and let κ_s be the neighbor-vertex design. Then*

$$\mathrm{mineff}\left(\kappa_s|\mathbb{O}\right) = \begin{cases} \min\left\{\frac{4}{m^2}\left(-2s\lfloor s\rfloor - s + \lfloor s\rfloor + \lfloor s\rfloor^2 + sm\right), \frac{s}{m}\right\} & \text{if } m \text{ is even} \\ \min\left\{\frac{4}{(m+1)(m-1)}\left(-2s\lfloor s\rfloor - s + \lfloor s\rfloor + \lfloor s\rfloor^2 + sm\right), \frac{s}{m}\right\} & \text{if } m \text{ is odd} \end{cases}$$

The next corollaries give the $\mathbb{O}$-minimal efficiency of the two most important Kiefer's designs.

Theorem 49 *Let $m > 1$ and let $\xi^*_{-\infty}$ be the E-optimal design for the model $(f, \mathfrak{X})$ which is given in Theorem 46. Then*

$$\mathrm{mineff}\left(\xi^*_{-\infty}|\mathbb{O}\right) = \begin{cases} 1/2 & \text{if } m \text{ is even} \\ (m+1)/(2m) & \text{if } m \text{ is odd} \end{cases}$$

Theorem 50 *([9]) Let $m > 1$ and let ξ^*_0 be a D-optimal design for the model $(f, \mathfrak{X})$. Then*

$$\mathrm{mineff}\left(\xi^*_0|\mathbb{O}\right) = \begin{cases} (m+2)/(2m+2) & \text{if } m \text{ is even} \\ (m+1)/(2m) & \text{if } m \text{ is odd} \end{cases}$$

Therefore, the $\mathbb{O}$-minimal efficiency of the E- and D-optimal designs is at least 50% and it converges to 50% with dimension m increasing to infinity.

We will show that, with an exception of the case $m \bmod 4 = 2$, the $\mathbb{O}$-maximin efficient design for $(f, \mathfrak{X})$ is the neighbor-vertex design κ_s with $s = \frac{3}{4}m$ and its $\mathbb{O}$-minimal efficiency is exactly 3/4.

Theorem 51 *Let $m \in \mathfrak{N}$. Set $s = 1$ if $m = 1$ and*

$$\begin{array}{ll} s = 3m/4 & \text{if } m \bmod 4 \in \{0,1,3\}, \ m \neq 1 \\ s = 3m/4 - 1/(3m) & \text{if } m \bmod 4 = 2 \end{array}$$

Then the neighbor vertex design κ_s is $\mathbb{O}$-maximin efficient for the model $(f, \mathfrak{X})$. Moreover

$$\operatorname{mineff}(\kappa_s|\mathbb{O}) = \begin{cases} 3/4 & \text{if } m \bmod 4 \in \{0,1,3\}, m \neq 1 \\ 3/4 - 1/(3m^2) & \text{if } m \bmod 4 = 2 \end{cases}$$

Proof. Proposition 44 entails that for some $s \in [0, m]$ the neighbor-vertex design κ_s is $\mathbb{O}$-minimax efficient from the reason that the criterion of $\mathbb{O}$-minimal efficiency is orthogonally invariant. Clearly, the value of s which gives the $\mathbb{O}$-minimax efficient design maximizes the minima in Theorem 48.

Let m be even. Then we need to maximize the function $\min\{q_0(m,s), s/m\}$ on $[0,m]$, where $q_0(m,s) = \frac{4}{m^2}\left(-2s\lfloor s\rfloor - s + \lfloor s\rfloor + \lfloor s\rfloor^2 + sm\right)$. Notice that $q_0(m, m/2) = 1$, $q_0(m,m) = 0$, and that $q_0(m,\cdot)$ is decreasing on $[m/2, m]$. Therefore, the maximum of $\min\{q_0(m,s), s/m\}$ is attained at the point $s \in [m/2, m]$ which solves the equation $q_0(m,s) = s/m$. One can verify that the solution is $s = \frac{3}{4}m$ if $m \bmod 4 = 0$ and $s = \frac{3}{4}m - \frac{1}{3}m^{-1}$ if $m \bmod 4 = 2$.

If m is odd, then we need to maximize $\min\{q_1(m,s), s/m\}$ on $[0,m]$, where $q_1(m,s) = \frac{4}{(m+1)(m-1)}\left(-2s\lfloor s\rfloor - s + \lfloor s\rfloor + \lfloor s\rfloor^2 + sm\right)$. Since $q_0(m,(m+1)/2) = 1$, $q_0(m,m) = 0$, and $q_0(m,\cdot)$ is decreasing on $[(m+1)/2, m]$, we need to find the solution $s \in [(m+1)/2, m]$ which solves $q_1(m,s) = s/m$. Again, it is straightforward to verify that the solution is $s = \frac{3}{4}m$.

■

Chapter 9

MULTIVARIATE LINEAR REGRESSION OF THE FIRST DEGREE WITH A CONSTANT TERM

9.1 Definition of the model and j-vertex designs

Consider the d-way linear regression model of the first degree with a nonzero intercept term given by the formula

$$y = x_1\beta_1 + ... + x_d\beta_d + c\beta_{d+1} + \varepsilon,\ x_1, ..., x_d \in \{0,1\}$$

where c is a known positive constant.

Suppose that $\beta_1, ..., \beta_d$ represent unknown weights, and the components of x mean the presence or absence of items in a weighing (similarly as in the model from the previous chapter). Then β_{d+1} can represent an unknown constant bias of the spring balance, caused for instance by an additional weight of different character, which is necessarily present in all the weighings. Notice that the constant c basically quantifies our interest about the intercept term compared to $\beta_1, ..., \beta_d$ in the sense that a small value of c indicates that the intercept term is important, while a large value of c means that the estimation of the parameters $\beta_1, ..., \beta_d$ is of primary interest.

In the standard notation used in this work, the experimental domain is $\mathfrak{X} = \{0,1\}^d$, the set of all designs is Ξ, and the $m = d+1$ dimensional vector of regression functions is

$$f : \mathfrak{X} \to \mathfrak{R}^{d+1};\ f(x_1, ..., x_d) = (x_1, ..., x_d, c)^T$$

Let $\mathfrak{X}_j$ be the set of all unit cube vertices from $\mathfrak{X}$ having j components equal to 1 and $d-j$ components equal to 0. Next, let κ_j be the j-vertex design - the uniform probability on $\mathfrak{X}_j$. In the sequel, we will construct designs in the class Ξ_* of all convex combinations of j-vertex designs. The next proposition justifies this restriction.

Proposition 52 *For any $\xi \in \Xi$ there exists a design $\overline{\kappa} \in \Xi_*$, such that*

$$\Phi(\mathbf{M}(\overline{\kappa})) \geq \Phi(\mathbf{M}(\xi)) \text{ for all } \Phi \in \mathbb{O}$$

Therefore, for any orthogonally invariant criterion Φ, some convex combination of j-vertex designs is Φ-optimal.

Proof. Let $\xi \in \Xi$ be an arbitrary design. We will show that the symmetrization $\overline{\kappa} \in \Xi_*$ of ξ which is given by

$$\overline{\kappa}\left(x\right)=\binom{d}{j}^{-1}\sum_{x^{/}\in\mathfrak{X}_{j}}\xi\left(x^{/}\right)\text{ for all }x\in\mathfrak{X}_{j},\ j=0,...,d$$

performs equally or better than ξ with respect to any $\Phi\in\mathbb{O}$.

Let $\mathbf{P}_i$, $i=1,...,d!$ be the permutation matrices of type $(d+1)\times(d+1)$, which permute the first d components, and leave the last component unchanged. Fix $j\in\{0,...,d\}$. The heart of the proof is based on geometric symmetries of the model, which can be algebraically stated in these two statements:

(i) The matrix $\sum_{i=1}^{d!}\mathbf{P}_i f(x)f^T(x)\mathbf{P}_i^T$ is the same for all $x\in\mathfrak{X}_j$;

(ii) The matrix $\sum_{x\in\mathfrak{X}_j}\mathbf{P}_i f(x)f^T(x)\mathbf{P}_i^T$ is the same for all $i=1,...,d!$.

The reason of (i) (or (ii)) is that different x'es (resp. i's) lead to sums with the same terms summed in a possibly different order. Using (i) with $\sum_{x\in\mathfrak{X}_j}\xi\left(x\right)=\sum_{x\in\mathfrak{X}_j}\overline{\kappa}\left(x\right)$ and then using (ii) with the fact that $\overline{\kappa}\left(x\right)$ is the same for all $x\in\mathfrak{X}_j$ we obtain:

$$\begin{gathered}\sum_{x\in\mathfrak{X}_j}\xi\left(x\right)\sum_{i=1}^{d!}\tfrac{1}{d!}\mathbf{P}_i f(x)f^T(x)\mathbf{P}_i^T=\sum_{x\in\mathfrak{X}_j}\overline{\kappa}\left(x\right)\sum_{i=1}^{d!}\tfrac{1}{d!}\mathbf{P}_i f(x)f^T(x)\mathbf{P}_i^T=\\=\sum_{i=1}^{d!}\tfrac{1}{d!}\sum_{x\in\mathfrak{X}_j}\overline{\kappa}\left(x\right)\mathbf{P}_i f(x)f^T(x)\mathbf{P}_i^T=\sum_{i=1}^{d!}\tfrac{1}{d!}\sum_{x\in\mathfrak{X}_j}\overline{\kappa}\left(x\right)f(x)f^T(x)=\\\sum_{x\in\mathfrak{X}_j}\overline{\kappa}\left(x\right)f(x)f^T(x)\end{gathered}$$

Therefore

$$\begin{gathered}\sum_{i=1}^{d!}\tfrac{1}{d!}\mathbf{P}_i\mathbf{M}(\xi)\mathbf{P}_i^T=\sum_{i=1}^{d!}\tfrac{1}{d!}\mathbf{P}_i\left(\sum_{j=0}^{d}\sum_{x\in\mathfrak{X}_j}\xi\left(x\right)f(x)f^T(x)\right)\mathbf{P}_i^T=\\=\sum_{j=0}^{d}\sum_{x\in\mathfrak{X}_j}\xi\left(x\right)\sum_{i=1}^{d!}\tfrac{1}{d!}\mathbf{P}_i f(x)f^T(x)\mathbf{P}_i^T=\sum_{j=0}^{d}\sum_{x\in\mathfrak{X}_j}\overline{\kappa}\left(x\right)f(x)f^T(x)=\mathbf{M}(\overline{\kappa})\end{gathered}$$

Finally, if $\Phi\in\mathbb{O}$, then from orthogonal invariance ($\mathbf{P}_i$ are orthogonal matrices!) and concavity of Φ we derive

$$\Phi(\mathbf{M}(\xi))=\sum_{i=1}^{d!}\tfrac{1}{d!}\Phi\left(\mathbf{P}_i\mathbf{M}(\xi)\mathbf{P}_i^T\right)\leq\Phi\left(\sum_{i=1}^{d!}\tfrac{1}{d!}\mathbf{P}_i\mathbf{M}(\xi)\mathbf{P}_i^T\right)=\Phi\left(\mathbf{M}(\overline{\kappa})\right)$$

The proof is complete. (It is evident that the proposition is even valid for the larger class of all *permutationally* invariant criteria.)

■

Suppose that $w=(w_0,...,w_d)^T$ is a vector of nonnegative weights summing to 1 and denote the convex combination of the j-vertex designs as

$$\overline{\kappa}_w=\sum_{j=0}^{d}w_j\kappa_j\in\Xi_*$$

It is easy to verify that the information matrix of $\overline{\kappa}_w$ has the following block form.

$$\mathbf{M}\left(\overline{\kappa}_w\right)=\begin{pmatrix}\sum_{j=0}^{d}w_j\mathbf{H}_j & \sum_{j=0}^{d}w_j\frac{cj}{d}\times\mathbf{1}_d\\ \sum_{j=0}^{d}w_j\frac{cj}{d}\times\mathbf{1}_d^T & c^2\end{pmatrix},\text{ where}$$

$$\mathbf{H}_j=\frac{j(d-j)}{d(d-1)}\mathbf{I}_d+\frac{j(j-1)}{d(d-1)}1_d1_d^T\text{ if }d>1\text{ and }\mathbf{H}_0=0,\ \mathbf{H}_1=1\text{ if }d=1.$$

The next proposition already leads us close to identification of optimal designs for criteria depending on eigenvalues.

Proposition 53 *Let $d \geq 2$, and let $w \in \mathfrak{R}^{d+1}$ be a vector of nonnegative weights which sum to 1. Define $u_1, ..., u_{d-1} \in \mathfrak{R}^{d+1}$ by*

$$\begin{aligned}
&u_1 = 2^{-1/2} \times (1, -1, 0, ..., 0)^T \\
&u_2 = 6^{-1/2} \times (1, 1, -2, 0, ..., 0)^T \\
&u_3 = 12^{-1/2} \times (1, 1, 1, -3, 0, ..., 0)^T \\
&\cdots \\
&u_{d-1} = \left(d - 1 + (d-1)^2\right)^{-1/2} \times (1, 1, 1, ..., 1-d, 0)^T
\end{aligned}$$

Then $u_1, ..., u_{d-1}$ form an orthonormal system of eigenvectors of the information matrix $\mathbf{M}(\overline{\kappa}_w)$. The common eigenvalue of $\mathbf{M}(\overline{\kappa}_w)$ corresponding to $u_1, ..., u_{d-1}$ is

$$b(w) = \sum_{j=0}^{d} w_j \frac{j(d-j)}{d(d-1)}$$

Moreover, the 2-dimensional eigenspace of $\mathbf{M}(\overline{\kappa}_w)$ orthogonal to $u_1, ..., u_{d-1}$ is generated by

$$\begin{aligned}
&u_d^* = d^{-1/2}(1, 1, 1, ..., 1, 0)^T \\
&u_{d+1}^* = (0, 0, 0, ..., 0, 1)^T
\end{aligned}$$

with corresponding eigenvalues of $\mathbf{M}(\overline{\kappa}_w)$ equal to the eigenvalues of the matrix

$$\begin{pmatrix} \frac{1}{d}\sum_{j=0}^{d} w_j j^2 & \frac{c}{\sqrt{d}}\sum_{j=0}^{d} w_j j \\ \frac{c}{\sqrt{d}}\sum_{j=0}^{d} w_j j & c^2 \end{pmatrix}$$

Proof. Checking that $u_1, ..., u_{d-1}$ are orthonormal eigenvectors corresponding to the eigenvalue $b(w)$ is lengthy, but elementary. It is also obvious that the orthonormal vectors u_d^* and u_{d+1}^* are both orthogonal to $\operatorname{span}(u_1, ..., u_{d-1})$. Let u_d and u_{d-1} be orthonormal eigenvectors of $\mathbf{M}(\overline{\kappa}_w)$ which belong to the eigenspace $\operatorname{span}(u_d^*, u_{d+1}^*)$. Consider the matrices $\mathbf{U} = (u_d, u_{d+1})$ and $\mathbf{U}^* = \left(u_d^*, u_{d+1}^*\right)$ of type $(d+1) \times 2$. Clearly, there is an orthogonal 2×2 matrix $\mathbf{V}$, such that $\mathbf{U}^*\mathbf{V} = \mathbf{U}$. The eigenvalues of $\mathbf{M}(\overline{\kappa}_w)$ which correspond to u_d and u_{d-1} are the (two) components of $\lambda\left(\mathbf{U}^T\mathbf{M}(\overline{\kappa}_w)\mathbf{U}\right)$. But

$$\lambda\left(\mathbf{U}^T\mathbf{M}(\overline{\kappa}_w)\mathbf{U}\right) = \lambda\left(\mathbf{V}^T\mathbf{U}^{*T}\mathbf{M}(\overline{\kappa}_w)\mathbf{U}^*\mathbf{V}\right) = \lambda\left(\mathbf{U}^{*T}\mathbf{M}(\overline{\kappa}_w)\mathbf{U}^*\right)$$

One can easily verify that

$$\mathbf{U}^{*T}\mathbf{M}(\overline{\kappa}_w)\mathbf{U}^* = \begin{pmatrix} \frac{1}{d}\sum_{j=0}^{d} w_j j^2 & \frac{c}{\sqrt{d}}\sum_{j=0}^{d} w_j j \\ \frac{c}{\sqrt{d}}\sum_{j=0}^{d} w_j j & c^2 \end{pmatrix}$$

■

9.2 The D-optimal designs

The aim of this section is to show that the design which distributes weights uniformly on $\mathfrak{X}$ is D-optimal.

Theorem 54 *Let $d \geq 1$. Let ξ_0^* be the uniform probability on $\mathfrak{X}$. Then ξ_0^* is D-optimal for the model $(f, \mathfrak{X})$. Moreover,*

$$\mathbf{M}(\xi_0^*) = \begin{pmatrix} \frac{1}{4}\mathbf{I}_d + \frac{1}{4}1_d 1_d^T & \frac{c}{2}1_d \\ \frac{c}{2}1_d^T & c^2 \end{pmatrix}$$

$$\lambda(\mathbf{M}(\xi_0^*)) = \left(\lambda_1, \frac{1}{4}, ..., \frac{1}{4}, \lambda_{d+1}\right)$$

where λ_1, λ_{d+1} ($\lambda_1 < \lambda_{d+1}$) are the roots of

$$4\lambda^2 - (4c^2 + d + 1)\lambda + c^2$$

Proof. Clearly, $\xi_0^* = \sum_{j=0}^d 2^{-d}\binom{d}{j}\kappa_j$. It is simple to check that the information matrix $\mathbf{M}_0 = \mathbf{M}(\xi_0^*)$ is the one which is given in the theorem, using the expressions for the information matrices of $\overline{\kappa}_w$ and the following basic combinatorial identities:

$$\textstyle\sum_{j=0}^d \binom{d}{j} = 2^d, \text{ next } \sum_{j=0}^d j\binom{d}{j} = d \times 2^{d-1} \text{ and } \sum_{j=0}^d j(j-1)\binom{d}{j} = d(d-1) \times 2^{d-2}$$

For $d = 1$, the vector of eigenvalues of $\mathbf{M}_0$ can be directly calculated and for $d \geq 2$ it can be derived from Proposition 53.

Next, we need to show that the roots λ_1, λ_{d+1} satisfy $\lambda_1 \leq 1/4 \leq \lambda_{d+1}$. Firstly, it is clear that the smaller λ_1 is at most $\frac{c^2}{1+4c^2}$, because in the opposite case the minimal eigenvalue of $\mathbf{M}_0$ would be higher than the E-optimal value, which is impossible. Hence, $\lambda_1 < 1/4$.

On the other hand, the minimum of the polynomial $4\lambda^2 - (4c^2 + d + 1)\lambda + c^2$ is in the point $(4c^2 + d + 1)/8 > 1/4$, which means that the larger root is $\lambda_{d+1} > 1/4$. (The roots λ_1, λ_{d+1} can be stated explicitly, but the formulae are long and we can prove the ordering from the implicit description as well.)

The last step is to prove that ξ_0^* is D-optimal. Take an arbitrary point $x = \begin{pmatrix} x_0^T & c \end{pmatrix}^T \in \mathfrak{X}$, where $x_0 \in \{0, 1\}^d$. It is simple to verify that

$$x^T \mathbf{M}_0^{-1} x = \begin{pmatrix} x_0^T & c \end{pmatrix} \begin{pmatrix} 4\mathbf{I}_d & -\frac{2}{c}1_d \\ -\frac{2}{c}1_d^T & \frac{d+1}{c^2} \end{pmatrix} \begin{pmatrix} x_0 \\ c \end{pmatrix} = 4x_0^T x_0 - 4x_0^T 1_d + (d+1) = d+1$$

The previous equality means that $\max_{x \in \mathfrak{X}} x^T \mathbf{M}_0^{-1} x = d + 1 = m$, which proves D-optimality of ξ_0^* by the equivalence theorem (see e.g. [17], p. 117).

■

9.3 The E-optimal designs

In this section, we will construct E-optimal designs for the model $(f, \mathfrak{X})$ of any degree. Firstly, we will find the E-optimal design for the case $d = 1$.

Proposition 55 *Let $d = 1$ and let*

$$\xi_{-\infty}^{*} = \frac{1+2c^2}{1+4c^2}\kappa_0 + \frac{2c^2}{1+4c^2}\kappa_1$$

Then $\xi_{-\infty}^{*}$ is the unique E-optimal design. Moreover,

$$\mathbf{M}\left(\xi_{-\infty}^{*}\right) = \frac{c^2}{1+4c^2}\begin{pmatrix} 2 & 2c \\ 2c & 1+4c^2 \end{pmatrix}$$

$$\lambda\left(\mathbf{M}\left(\xi_{-\infty}^{*}\right)\right) = \left(\frac{c^2}{1+4c^2}, \frac{2c^2+4c^4}{1+4c^2}\right)^T$$

Proof. Suppose that $d = 1$. The proposition can be proved either by Lemma 3.1. in [5], or using elementary calculus as follows. Consider an arbitrary design $\xi \in \Xi$ and denote $w = \xi(1) \in [0, 1]$. It is then straightforward to show that

$$\mathbf{M}(\xi) = \begin{pmatrix} w & wc \\ wc & c^2 \end{pmatrix} \text{ and } \lambda_1\left(\mathbf{M}(\xi)\right) = \tfrac{1}{2}w + \tfrac{1}{2}c^2 - \tfrac{1}{2}\sqrt{\left(1+4c^2\right)w^2 - 2c^2w + c^4}$$

The proof can be closed noticing that λ_1 is a smooth function of the weight w and checking that $w^* = \frac{2c^2}{1+4c^2}$ is a single stationary point on the interval $(0, 1)$.
■

Using the previous proposition and results of Chapter 5, we can find an E-optimal design for all degrees of the model.

Theorem 56 *If d is even let*

$$\xi_{-\infty}^{*} = \frac{d+2c^2}{d(1+4c^2)}\kappa_0 + \frac{(d-1)4c^2}{d(1+4c^2)}\kappa_{d/2} + \frac{2c^2}{d(1+4c^2)}\kappa_d$$

and if d is odd let

$$\xi_{-\infty}^{*} = \frac{(d+1)+2c^2}{(d+1)(1+4c^2)}\kappa_0 + \frac{2dc^2}{(d+1)(1+4c^2)}\left(\kappa_{\frac{d-1}{2}} + \kappa_{\frac{d+1}{2}}\right) + \frac{2c^2}{(d+1)(1+4c^2)}\kappa_d$$

Then $\xi_{-\infty}^{*}$ is an E-optimal design and

$$\mathbf{M}\left(\xi_{-\infty}^{*}\right) = \frac{c^2}{1+4c^2} \times \begin{pmatrix} \mathbf{I}_d + 1_d 1_d^T & 2c1_d \\ 2c1_d^T & 1+4c^2 \end{pmatrix}$$

$$\lambda\left(\mathbf{M}\left(\xi_{-\infty}^{*}\right)\right) = \left(\frac{c^2}{1+4c^2}, \ldots, \frac{c^2}{1+4c^2}, \frac{(d+1)c^2+4c^4}{1+4c^2}\right)^T$$

Proof. The form of the information matrix of $\xi^*_{-\infty}$ can be easily derived from the expressions for the information matrices of the designs κ_w. Next, the eigenvalues of $\mathbf{M}\left(\xi^*_{-\infty}\right)$ can be calculated from Proposition 53. The only nontrivial fact is that $\xi^*_{-\infty}$ is E-optimal.

For $d = 1$, the theorem is identical to Proposition 55. Suppose that $d \geq 2$. Consider the 2-dimensional orthogonal submodel of $(f, \mathfrak{X})$, which we obtain by deleting the first $d-1$ components of f, i.e. the orthogonal submodel $(g, \mathfrak{X})$ where $g = \mathbf{U}^T f$ and the entries of $\mathbf{U} \in \mathcal{U}_{d+1,2}$ are given by the equalities: $(\mathbf{U})_{ij} = 1$ if $(i,j) \in \{(d,1),(d+1,2)\}$, and $(\mathbf{U})_{ij} = 0$ otherwise.

Evidently, the model $(g, \mathfrak{X})$ has the same Elfving set as the *two*-dimensional version of the model $(f, \mathfrak{X})$, i.e. for $d = 1$. Hence, Propositions 21 and 55 imply that the E-optimal value of $(g, \mathfrak{X})$ is $v_{g,\mathfrak{X}}(1) = c^2\left(1+4c^2\right)^{-1}$. Therefore

$$\Phi_{E_1}(\mathbf{M}_{f,\mathfrak{X}}\left(\xi^*_{-\infty}\right)) = \tfrac{c^2}{1+4c^2} = v_{g,\mathfrak{X}}(1)$$

Consequently, $\xi^*_{-\infty}$ is E-optimal by Proposition 17.

■

Using the methods developed in Chapter 5, it can also be shown that the E-optimal information matrix is unique for all dimensions d, and the E-optimal design is unique for $d = 1, 2$. It turns out that there is a multitude of distinct E-optimal designs for $d \geq 3$. Naturally, under certain practical circumstances, the E-optimal designs do not have to be equally suitable. For instance, we can have requirements on the number of "items in one weighing" and some of the E-optimal designs would comply to these restrictions, while others would not. However, this is a nontrivial problem, solution of which is not essential for this work.

Notice also that if $c \to \infty$, that is if we focus on estimation of $\beta_1, ..., \beta_d$, then the E-optimal design tends to put the mass $1/2d$ to the extreme vertex designs κ_0 and κ_d and the mass $(d-1)/d$ to the middle vertex design $\kappa_{d/2}$ (for an even d; the behavior for an odd d is similar). As can be verified using Proposition 53 and Theorem 54, this "limit" E-optimal design is one of more possible D-optimal designs.

9.4 Bounds on the E_k-optimal values

For the model in consideration, it seems to be difficult to find the exact E_k-optimal values, except of some special cases as $k = 1$ or $k = d+1$. Nevertheless, ideas from Chapter 5 allow us to find upper bounds on the E_k-optimal values, and consequently lower bounds on the $\mathbb{O}$-minimal efficiency.

Suppose that $d \geq 2$ and consider $u_1, ..., u_{d-1} \in \mathfrak{R}^{d+1}$ as defined in Proposition 53. Set

$$u_d^{/} = \left(4c^2 d + d^2\right)^{-1/2} \times (2c, 2c, ..., 2c, -d)^T$$

The vectors $u_1, ..., u_{d-1}, u_d^{/}$ are mutually orthogonal, normalized, and chosen such that

$$\mathbf{U} = \left(u_1, ..., u_{d-1}, u_d^{/}\right) \in \mathcal{U}_{d+1,d}$$

Notice that the projector $\mathbf{P} = \mathbf{U}^T\mathbf{U}$ projects orthogonally in the direction of the "central axis" $(1/2, ..., 1/2, c)^T$ of the Elfving set $\mathfrak{E}$ corresponding to the model $(f, \mathfrak{X})$.

Let $1 \leq k \leq d$. By Proposition 52 we know that there exists an E_k-optimal design $\overline{\kappa}_w$ that is a convex combination of the j-vertex designs defined by a vector of weights $w = (w_0, ..., w_d)^T$. It is straightforward to show that

$$\left(u_d^{/}\right)^T \cdot \mathbf{M}\left(\overline{\kappa}_w\right) \cdot u_d^{/} = \frac{c^2}{d^2 + 4dc^2} \times \sum_{j=0}^{d} w_j (2j - d)^2 =: b^*(w)$$

Therefore, Propositions 16 and 53 imply that

$$\Phi_{E_k}\left(\mathbf{M}\left(\overline{\kappa}_w\right)\right) \leq \Phi_{E_k}\left(\mathbf{U}^T \mathbf{M}\left(\overline{\kappa}_w\right) \mathbf{U}\right) \leq \Phi_{E_k}\begin{pmatrix} b(w) \times \mathbf{I}_{d-1} & 0_{d-1} \\ 0_{d-1}^T & b^*(w) \end{pmatrix}$$

Consequently, if $1 \leq k \leq d$, then we have the following upper bounds on the E_k-optimal values. (The maximum is taken with respect to all possible vectors w of weights.)

$$\begin{array}{ll} v(k) \leq \max_w \min\left\{kb(w), (k-1)b(w) + b^*(w)\right\} & \text{if } 1 \leq k \leq d-1 \\ v(k) \leq \max_w \left((d-1)b(w) + b^*(w)\right) & \text{if } k = d \end{array}$$

We can rewrite the previous inequalities into a form which does not require maximization over an m-dimensional simplex, as is shown in the following proposition.

Proposition 57 *The E_k-optimal values $v(k)$ of the model $(f, \mathfrak{X})$ satisfy*

$$\begin{array}{l} v(1) = \frac{c^2}{1+4c^2} \\ v(k) \leq \min_{q\in[0,1]} \max\limits_{j=0,...,d} \left\{\frac{(k-q)j(d-j)}{d(d-1)} + \frac{qc^2(2j-d)^2}{d^2+4dc^2}\right\} \textit{ if } d \geq 3 \textit{ and } 1 < k < d \\ v(d) \leq \max\limits_{j=0,...,d} \left\{\frac{j(d-j)}{d} + \frac{c^2(2j-d)^2}{d^2+4dc^2}\right\} \\ v(d+1) = d + c^2 \end{array}$$

Proof. The E-optimal value $v(1)$ comes from Theorem 56. Suppose that $d \geq 3$ and $1 < k < d$. We can write

$$\begin{array}{c} \max_w \min\left\{kb(w), (k-1)b(w) + b^*(w)\right\} \leq \\ \leq \max_w \min_{q\in[0,1]} \left((1-q)kb(w) + q\left((k-1)b(w) + b^*(w)\right)\right) \leq \\ \leq \min_{q\in[0,1]} \max_w \left((1-q)kb(w) + q\left((k-1)b(w) + b^*(w)\right)\right) \end{array}$$

The last inequality follows from Lemma 36.1 in [22]. As $b(w)$ and $b^*(w)$ depend linearly on the vector w of weights, the maximum is attained on the vertices of the $(d+1)$-dimensional unit simplex, that is on the basic unit vectors $e_1, ..., e_{d+1} \in \mathfrak{R}^{d+1}$. Consequently

$$\begin{array}{c} \max_w \min\left\{kb(w), (k-1)b(w) + b^*(w)\right\} \leq \\ \leq \min_{q\in[0,1]} \max\limits_{i=1,...,d+1} \left((1-q)kb(e_i) + q\left((k-1)b(e_i) + b^*(e_i)\right)\right) = \\ = \min_{q\in[0,1]} \max\limits_{i=1,...,d+1} \left((k-q)\, b(e_i) + qb^*(e_i)\right) \end{array}$$

We can use the expressions for the functions b and b^* to get the form of the bound given in the theorem. The bound for $v(d)$ can be proved analogously, and the T-optimal value $v(d+1)$ is based on the easy to verify fact that the T-optimal design is the singular measure on $(1, ..., 1, c)^T$.

■

For example if $d = 2$ then the previous proposition yields

$$v(2) \le \max\left\{\frac{c^2}{1+2c^2}, \frac{1}{2}, \frac{c^2}{1+2c^2}\right\} = \frac{1}{2}$$

Similarly, if $d = 3$ then we obtain

$$v(2) \le \min_{q\in[0,1]} \max\left\{\tfrac{3qc^2}{3+4c^2}, \tfrac{2-q}{3} + \tfrac{q}{3}\tfrac{c^2}{3+4c^2}\right\} = \begin{cases} \frac{2c^2}{4c^2+1} & \text{if } c \ge \frac{\sqrt{3}}{2} \\ \frac{1}{3}\frac{3+5c^2}{3+4c^2} & \text{if } c \le \frac{\sqrt{3}}{2} \end{cases}$$

$$v(3) \le \max\left\{\tfrac{3c^2}{3+4c^2}, \tfrac{2+3c^2}{3+4c^2}, \tfrac{3c^2}{3+4c^2}\right\} = \tfrac{2+3c^2}{3+4c^2}$$

In order to find the bound on $v(k)$ given by Proposition 57 for $d \ge 3$ and $1 < k < d$, we only need to minimize a (known) piecewise-linear convex function on the interval $[0, 1]$. Hence, the bounds can be mechanically calculated for a general dimension of the model.

If, for instance, $c = 1$, then we can compute and summarize the (bounds on) the values $v(k)$ in the table given below. (Notice that the lower bounds are based on the E-optimal designs.)

	d=1	d=2	d=3	d=4
k=1	1/5	1/5	1/5	1/5
k=2	2	$[2/5, 1/2]$	2/5	2/5
k=3	-	3	$[3/5, 5/7]$	$[3/5, 2/3]$
k=4	-	-	4	$[4/5, 1]$
k=5	-	-	-	5

Using Proposition 57, we can also derive very simple bounds on the E_k-optimal values (for $k \le d$), which do *not* depend on d and c.

Theorem 58 *Let $1 \le k \le d$. Then $v(k) \le k/4$.*

Proof. From Proposition 57 we see that

$$v(d) \le \max_{j=0,\ldots,d}\left\{\tfrac{j(d-j)}{d} + \tfrac{c^2(2j-d)^2}{4dc^2}\right\} = d/4$$

But Proposition 8 entails that the point $(k, v(k))$ must lie below the line connecting $(0, 0)$ and $(d, v(d))$. The inequality $v(k) \le k/4$ is now evident.

■

9.5 The $\mathbb{O}$-minimal efficiency of the E- and D-optimal designs

After proving the necessary auxiliary results in the previous section, we are able to formulate the following theorem about the $\mathbb{O}$-minimal efficiency of E-, and D-optimal designs.

Theorem 59 *Consider designs $\xi^*_{-\infty}$ and ξ^*_0 given in Theorems 56 and 54. Then*

$$\text{mineff}(\xi^*_{-\infty}|\mathbb{O}) = \frac{c^2\,(4c^2+1+2d)}{(c^2+d)\,(4c^2+1)}$$

$$\text{mineff}(\xi^*_0|\mathbb{O}) \geq \min\left\{\frac{1+4c^2}{d+1+4c^2}, \frac{d+2c^2}{2d+2c^2}\right\}$$

$$\text{mineff}(\xi^*_0|\mathbb{O}) \leq \min\left\{\frac{1+4c^2}{d+\frac{1}{1+4c^2}+4c^2}, \frac{d+2c^2}{2d+2c^2}\right\}$$

Proof. Using Theorems 55, 56, 58 and the T-optimal value $v(d+1) = d+c^2$ from Proposition 57 we obtain for all $1 \leq k \leq d$:

$$\text{eff}\,(\xi^*_{-\infty}|\Phi_{E_k}) \geq \frac{4c^2}{1+4c^2} \geq \frac{(4c^2+1+2d)\,c^2}{(1+4c^2)\,(c^2+d)} = \text{eff}\,(\xi^*_{-\infty}|\Phi_{E_{d+1}})$$

According to Theorem 11, this proves the formula for the $\mathbb{O}$-minimal efficiency of the E-optimal design $\xi^*_{-\infty}$.

Next, we will derive the bounds for the D-optimal design ξ^*_0. By Theorem 11 we need to find bounds on the E_1-, E_d- and E_{d+1}-efficiency of ξ^*_0.

By Theorem 54, the minimal eigenvalue λ_1 of $\mathbf{M}\,(\xi^*_0)$ is a root of $4\lambda^2-(d+1+4c^2)\lambda+c^2$. Therefore $\lambda_1 = \rho\,(\lambda_1)$, where the function $\rho : (0,\infty] \to \mathfrak{R}$ is defined by

$$\rho\,(\lambda) = c^2\,(d+1+4c^2-4\lambda)^{-1}$$

Notice, that ρ is increasing on $(0,\infty]$. Clearly, λ_1 is positive and, in the same time, less than the E-optimal value given by Theorems 55 and 56. The inequalities $\lambda_1 > 0$ and $\lambda_1 < c^2\,(1+4c^2)^{-1}$ then entail:

$$\lambda_1 = \rho\,(\lambda_1) > \rho(0) = c^2\,(d+1+4c^2)^{-1}$$
$$\lambda_1 = \rho\,(\lambda_1) < \rho(c^2\,(1+4c^2)^{-1}) = c^2\left(d+(1+4c^2)^{-1}+4c^2\right)^{-1}$$

The E-optimal (i.e. E_1-optimal) value and the previous inequalities give

$$\text{eff}(\xi^*_0|\Phi_{E_1}) = \frac{\lambda_1}{c^2\,(1+4c^2)^{-1}} \in \left(\frac{1+4c^2}{d+1+4c^2}, \frac{1+4c^2}{d+\frac{1}{1+4c^2}+4c^2}\right)$$

Moreover, Theorem 58 implies $v_c^{(d)}(d) \leq d/4$, which means

$$\mathrm{eff}(\xi_0^*|\Phi_{E_d}) \geq \left(\frac{c^2}{d+1+4c^2} + \frac{d-1}{4}\right) : (d/4) \geq \frac{1+4c^2}{d+1+4c^2}$$

where the second inequality is easy to show by direct algebraic manipulations. Finally, as the T-optimal (E_{d+1}-optimal) value is $v(d+1) = d + c^2$ we can write

$$\mathrm{eff}(\xi_0^*|\Phi_{E_{d+1}}) = \frac{\mathrm{tr}\,\mathbf{M}\,(\xi_0^*)}{d+c^2} = \frac{2d+4c^2}{4d+4c^2}$$

Consequently, the value $\mathrm{mineff}(\xi_0^*|\mathbb{O}) = \min_{k\in\{1,d,d+1\}} \mathrm{eff}(\xi_0^*|\Phi_{E_k})$ is between the bounds given in the theorem.

■

Although we have not the exact value of $\mathrm{mineff}(\xi_0^*|\mathbb{O})$ identified, the bounds given in Theorem 59 are very tight, as is also obvious from the illustrative graphs in Figures 3 and 4 for selected degrees $d = 2$ and $d = 8$. Notice also, that there exist values of d and c such that $\mathrm{mineff}(\xi_{-\infty}^*|\mathbb{O})$ is greater than $\mathrm{mineff}(\xi_0^*|\mathbb{O})$ and vice versa.

In the last part of this section, we will briefly point out some implications of Theorem 59 for the limiting cases of c and d.

Under the assumption that $c \to \infty$ and d is fixed, the $\mathbb{O}$-minimal efficiencies of E- and D-optimal designs converge to 1. This means that if the parameter of intercept is unknown, but of negligible interest, then E- and D-optimal designs have both very high performance with respect to all orthogonally invariant criteria.

If $d \to \infty$ and c is fixed, then $\mathrm{mineff}(\xi_0^*|\mathbb{O})$ converges to 0, while the $\mathbb{O}$-minimal efficiency of the E-optimal design remains bounded from below by $\frac{2c^2}{4c^2+1}$. Consequently, for a large value of d and a moderate c, the E-optimal design should be preferred to the D-optimal design, provided that we require a design which is robust with respect to selection of a criterion from the class $\mathbb{O}$.

The last observation has a theoretical value. If $c \to 0$ and d is fixed, then the upper bound on $\mathrm{mineff}(\xi_0^*|\mathbb{O})$ converges to $1/(d+1) = 1/m$. Hence, Theorem 32 gives the strongest lower bound on the $\mathbb{O}$-minimal efficiency of D-optimal designs which depends only on the number m of parameters.

Chapter 10

QUADRATIC, CUBIC AND BIQUADRATIC REGRESSION ON THE INTERVAL $[-1, 1]$

10.1 Definition of the model and the E_k-optimal values

Consider the polynomial regression of degree d on the experimental domain $\mathfrak{X} = [-1, 1]$ given by the model equation

$$y = \beta_1 + \beta_2 x + ... + \beta_{d+1} x^d + \varepsilon$$

In the notation of this article, the vector of unknown parameters of interest $\beta = (\beta_1, \beta_2, ..., \beta_{d+1})^T$ is $m = d + 1$ dimensional and the vector of regression functions is $f(x) = (1, x, ..., x^d)^T$.

We will analyze this model for degrees $d \in \{1, 2, 3, 4\}$ with the aim to evaluate the minimal efficiency of Φ_p-optimal designs, $p \in [-\infty, 1]$, with respect to the class $\mathbb{O}$ of all orthogonally invariant criteria. As special cases, we will obtain the $\mathbb{O}$-minimal efficiency for the D-, A-, and E-optimal designs. Moreover, for the quadratic regression ($d = 2$), we will identify the design which is $\mathbb{O}$-maximin efficient.

Firstly, we need to find the optimal values for the criteria of E_k-optimality. It turns out that the E_k-optimal designs for degrees $d = 1, 2, 3, 4$, and for $k = 1, ..., d+1$ can be found explicitly. For $k = 1$, that is for the ordinary E-optimality, the optimal designs are known (see [20] or [19] p. 232-237), and we denote them by $\zeta_1^{(d)}$. In particular, the simplest design $\zeta_1^{(1)}$ assigns the weight $\frac{1}{2}$ to -1 and 1. Next, by $\zeta_3^{(4)}$ we denote the design which assigns the weight 1/6 to -1,1, and the weight 2/3 to 0. Using Theorem 6, it is simple to verify that for any considered combination of d and k, some of the five designs described (i.e. $\zeta_1^{(1)}, ..., \zeta_1^{(4)}$ or $\zeta_3^{(4)}$) is E_k-optimal. The E_k-optimal designs and the corresponding optimal values are summarized in the following table.

	d=1	d=2	d=3	d=4
k=1	$\zeta_1^{(1)}; 1$	$\zeta_1^{(2)}; 1/5$	$\zeta_1^{(3)}; 1/25$	$\zeta_1^{(4)}; 1/129$
k=2	$\zeta_1^{(1)}; 2$	$\zeta_1^{(1)}; 1$	$\zeta_1^{(2)}; 1/5$	$\zeta_1^{(3)}; 1/25$
k=3	-	$\zeta_1^{(1)}; 3$	$\zeta_1^{(1)}; 2$	$\zeta_3^{(4)}; 1/3$
k=4	-	-	$\zeta_1^{(1)}; 4$	$\zeta_1^{(1)}; 2$
k=5	-	-	-	$\zeta_1^{(1)}; 5$

Notice that in the case of line regression ($d = 1$) the design $\zeta_1^{(1)}$ is E_k-optimal for both $k = 1, 2$. This means that $\zeta_1^{(1)}$ is optimal with respect to all orthogonally invariant criteria.

10.2 The $\mathbb{O}$-minimal efficiency of Φ_p-optimal designs

The E_k-optimal values allow us to compute the $\mathbb{O}$-minimal efficiency for the Φ_p-optimal designs, $p \in [-\infty, 1]$. For polynomial regression on $[-1, 1]$, the $E \approx \Phi_{-\infty}$, $A \approx \Phi_{-1}$, and $D \approx \Phi_0$-optimal designs are known (see e.g. [19] Chapter 9). For these designs, the following tables give the E_k-efficiencies. According to Theorem 10, the minimum of these $d + 1$ efficiencies equals to the $\mathbb{O}$-minimal efficiency.

eff	E_1	E_2	E_3	$\mathbb{O}$-minimal
D	0.730745	0.812816	0.777778	0.730745
A	0.954915	0.690983	0.666667	0.666667
E	1.000000	0.600000	0.600000	0.600000

d=2

eff	E_1	E_2	E_3	E_4	$\mathbb{O}$-minimal
D	0.744733	0.717848	0.608890	0.656000	0.608890
A	0.967451	0.721081	0.432425	0.523166	0.432425
E	1.000000	0.638861	0.396386	0.501250	0.396386

d=3

eff	E_1	E_2	E_3	E_4	E_5	$\mathbb{O}$-minimal
D	0.738857	0.714339	0.683360	0.603928	0.577976	0.577976
A	0.969005	0.709550	0.637469	0.443494	0.448069	0.443494
E	1.000000	0.627669	0.603550	0.433000	0.441860	0.433000

d=4

For an arbitrary $p \in [-\infty, 1]$, the Φ_p-optimal design can be computed using general iterative methods (see [17] Chapter V). The graphs in Figures 5, 6, 7 exhibit the numerically computed E_k-efficiencies, and the $\mathbb{O}$-minimal efficiency of Φ_p-optimal designs. The parameter r, which corresponds to the horizontal axis, relates to the parameter p via the function $p(r) = \frac{2r}{1+r}$ for $r \in (-1, 1]$ and $p(r) = -\infty$ for $r = -1$. Hence, E-, A-, D- and T-optimality correspond to $r = -1, -1/3, 0$, resp. 1. Notice also that the function $p(\cdot)$ is chosen such that $p(r)+p(-r) = p(r)p(-r)$, which means that $p(r)$ and $p(-r)$ are conjugate numbers.

From the graphs of the minimal efficiency with respect to $\mathbb{O}$ we see that the D-optimal design performs well, yet it does not maximize the $\mathbb{O}$-minimal efficiency even within the class of Φ_p-optimal designs.

10.3 The $\mathbb{O}$-maximin efficient design for quadratic regression

In general, it is difficult to find the $\mathbb{O}$-maximin efficient design without resorting to numerical procedures for maximization of a nondifferentiable function. Nevertheless, for the case of the quadratic regression, we can construct the maximin efficient design explicitly:

Theorem 60 *([8]) Let ξ be the design which assigns the weight $w = \frac{46}{251} + \frac{15}{502}\sqrt{22} \doteq 0.32342$ to the points -1,1 and the weight $1 - 2w \doteq 0.35316$ to the point 0. Then ξ is maximin efficient with respect to $\mathbb{O}$ for the quadratic regression on $[-1, 1]$. The $\mathbb{O}$-minimal efficiency of ξ is $\frac{145}{251} + \frac{10}{251}\sqrt{22} \doteq 0.76456$.*

Proof. It is simple to verify that the eigenvalues of $\mathbf{M} = \mathbf{M}(\xi)$ (cf. [19] p.333) are

$$\lambda_1(\mathbf{M}) = \tfrac{29}{251} + \tfrac{2}{251}\sqrt{22} \doteq 0.15291,\ \lambda_2(\mathbf{M}) = \tfrac{92}{251} + \tfrac{15}{251}\sqrt{22} \doteq 0.64684,$$
$$\lambda_3(\mathbf{M}) = \tfrac{314}{251} + \tfrac{13}{251}\sqrt{22} \doteq 1.49393$$

We already know that the optimal values for Φ_{E_k}, $k = 1, 2, 3$ are $v(1) = 1/5$, $v(2) = 1$, and $v(3) = 3$, therefore

$$\begin{aligned}
&\Phi_{E_1}(\mathbf{M})/v(1) = 5\lambda_1(\mathbf{M}) = \tfrac{145}{251} + \tfrac{10}{251}\sqrt{22} \doteq 0.76456\\
&\Phi_{E_2}(\mathbf{M})/v(2) = \lambda_1(\mathbf{M}) + \lambda_2(\mathbf{M}) = \tfrac{121}{251} + \tfrac{17}{251}\sqrt{22} \doteq 0.79975\\
&\Phi_{E_3}(\mathbf{M})/v(3) = \tfrac{1}{3}\left\{\lambda_1(\mathbf{M}) + \lambda_2(\mathbf{M}) + \lambda_3(\mathbf{M})\right\} = \tfrac{145}{251} + \tfrac{10}{251}\sqrt{22} \doteq 0.76456
\end{aligned}$$

Thence the $\mathbb{O}$-minimal efficiency of ξ is

$$\Phi_{\mathbb{O}}(\mathbf{M}) = \min_{k=1,2,3} \widetilde{\Phi}_{E_k}(\mathbf{M})/v(k) = \tfrac{145}{251} + \tfrac{10}{251}\sqrt{22} \doteq 0.76456$$

The eigenvalues of $\mathbf{M}$ are mutually distinct, hence by the discussion following Proposition 4 we know that Φ_{E_k}'s are differentiable in $\mathbf{M}$, which means that there exist unique gradients of $\widetilde{\Phi}_{E_k}$ in $\mathbf{M}$ for all k. Moreover, as the active set used in Proposition 13 is $\mathfrak{I} = \{1, 3\}$, we see that the subgradients of $\widetilde{\Phi}_{\mathbb{O}}$ in $\mathbf{M}$ are of the form

$$\mathbf{Y} = \alpha\nabla\widetilde{\Phi}_{E_1}(\mathbf{M})/v(1) + (1-\alpha)\nabla\widetilde{\Phi}_{E_3}(\mathbf{M})/v(3),\ \alpha \in [0, 1].$$

In the sequel, we shall use the subgradient $\mathbf{Y}$ which corresponds to $\alpha = \frac{11}{251} + \frac{285}{5522}\sqrt{22} \doteq 0.28591$. From Proposition 4, it can be calculated that

$$\nabla\widetilde{\Phi}_{E_1}(\mathbf{M}) = \begin{pmatrix} a & 0 & b \\ 0 & 0 & 0 \\ b & 0 & c \end{pmatrix},\ \text{where } a = \tfrac{59+12\sqrt{22}}{313}, b = \tfrac{-90-13\sqrt{22}}{313}, c = \tfrac{254-12\sqrt{22}}{313}.$$

Moreover, $\widetilde{\Phi}_{E_3}$ is simply the trace, therefore $\nabla\widetilde{\Phi}_{E_3}(\mathbf{M}) = \mathbf{I}_3$. Using algebraic simplifications and elementary calculus we finally obtain

$$f^T(x)\mathbf{Y}f(x) = \tfrac{220+145\sqrt{22}}{5522} \times \left(7x^4 - 7x^2 + \sqrt{22}\right)$$
$$\max_{x\in[0,1]} f^T(x)\mathbf{Y}f(x) = \tfrac{145}{251} + \tfrac{10\sqrt{22}}{251} = \Phi_{\mathbb{O}}(\mathbf{M})$$

By Theorem 14, this proves that ξ is the $\mathbb{O}$-maximin efficient design.
$\blacksquare$

It can be shown that in the case of quadratic regression, the $\mathbb{O}$-maximin efficient design ξ must be Φ_{p_ξ}-optimal for some $p_\xi \in [-\infty, 1]$. (More generally, if $d = 2$ then *any* design which is optimal with respect to some $\Phi \in \mathbb{O}$ is also Φ_p-optimal for some p; see the considerations in [19] p. 334. On the other hand, our preliminary numerical computations suggest that for $d > 2$ the $\mathbb{O}$-maximin efficient design does *not* belong to the class of Φ_p-optimal designs). One can calculate that $p_\xi \doteq -0.0648$ (i.e. $r_\xi \doteq -0.0314$; cf. with Figure 5).

At the end of this chapter, let us use the quadratic regression to demonstrate the methods of Section 4.3 leading to a convex combination $\overline{\xi}_{w^*}$ of E_k-optimal designs, proposed with the intention to guarantee a stable performance under all orthogonally invariant criteria.

To calculate the vector of weights w^* we need to solve a linear programming problem: find $\max y$, where

$$x = (w_1, w_2, w_3, \delta_1, \delta_2, \delta_3, y)^T \in \mathfrak{R}^7_+$$

$$\begin{pmatrix} 1 & 0 & 0 & -1 & 0 & 0 & -1 \\ 3/5 & 1 & 1 & 0 & -1 & 0 & -1 \\ 3/5 & 1 & 1 & 0 & 0 & -1 & -1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} x = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

A solution of this problem is $x^* = (5/7, 2/7, 0, 0, 0, 0, 5/7)^T$ (calculated using the program R). Hence, the design

$$\overline{\zeta}_{w^*} = \frac{5}{7} \times \zeta_1^{(2)} + \frac{2}{7} \times \zeta_1^{(1)} = \begin{pmatrix} -1 & 0 & 1 \\ 2/7 & 3/7 & 2/7 \end{pmatrix}$$

has $\mathbb{O}$-minimal efficiency bounded below by the last component of x^* which is equal to $5/7 \doteq 0.7143$. (In fact, one can check that $5/7$ is the exact value of this efficiency.) This is substantially more than the $\mathbb{O}$-minimal efficiency of the E-optimal design we used for construction of $\overline{\zeta}_{w^*}$, and only slightly less than the $\mathbb{O}$-minimal efficiency of the known $\mathbb{O}$-maximin efficient design given by Theorem 60.

Chapter 11

IMPROVING PERFORMANCE OF ALGORITHMS FOR CONSTRUCTION OF D-OPTIMAL DESIGNS

11.1 Deletion of points which do not support a D-optimal design

The problem of numerical construction of D-optimal designs has gained much attention in the experimental design literature. The main problem of existing iterative algorithms (see e.g. [17], Chapter V) is their slow convergence, especially for a large dimension of the parameter. Also, the support of the design measures obtained in the iterative process does not have a tendency to shrink, that is the output of a program which implements these algorithms contains many points with small weights, or groups of points, which are very close together.

To address this problem, we will describe a geometrically based method published in [7] which allows us to remove some unnecessary points of the experimental domain, that is some of the points of $\mathfrak{X}$, which can not support any D-optimal design measure.

We remark that the iterative algorithms used for construction of a D-optimal design need to scan the experimental domain in every iteration. (This is best seen if $\mathfrak{X}$ is finite.) Using the methods of this chapter, we are able to restrict our attention to a set which is smaller than $\mathfrak{X}$ and, as a rule, gain an increase in the computational speed as well as obtain the final design in a compact, small-support form.

One possible approach to this problem is to delete the points $x \in \mathfrak{X}$, such that $f(x)$ is not an extreme point of the Elfving set of the m-dimensional model $(f, \mathfrak{X})$ in consideration (cf. [27], [17] p.56 see also Proposition 21). However, in majority of commonly used models this method removes only small parts of $\mathfrak{X}$, and does not help us use the knowledge gained during the iterative process of computation of a design. Moreover, the method is difficult from the computational point of view. The method proposed in this chapter is completely different and does not have these disadvantages.

The main idea of the method is formulated in the following simple proposition:

Proposition 61 *([7]) Let $\mathcal{P} \subseteq \mathcal{S}^m_{++}$ be a set containing the D-optimal information matrix $\mathbf{M}_0$. If $\sup_{\mathbf{M}\in\mathcal{P}} f^T(x)\mathbf{M}^{-1}f(x) < m$ for some $x \in \mathfrak{X}$, then x does not support any D-optimal design, i.e. for all D-optimal designs ξ_0^*:*

$$\xi_0^*\{x \in \mathfrak{X} : \sup_{\mathbf{M}\in\mathcal{P}} f^T(x)\mathbf{M}^{-1}f(x) < m\} = 0$$

In particular, if $\mathbf{M}_0 \in \mathcal{P} = \operatorname{conv}\{\mathbf{Q}_1, ..., \mathbf{Q}_r\}$ *for some* $\mathbf{Q}_1, ..., \mathbf{Q}_r \in \mathcal{S}^m_{++}$*, and if* $\max_{i=1,...,r} f^T(x)\mathbf{Q}_i^{-1} f(x) < m$*, then* $x \in \mathfrak{X}$ *does not support any D-optimal design.*

Proof. If ξ_0^* is a D-optimal design, then ξ_0^*- almost all points from $\mathfrak{X}$ satisfy the condition $f^T(x)\mathbf{M}^{-1}(\xi_0^*) f(x) = m$ (cf. [32], Theorem 1c), which entails the first part of the proposition. The second part is a consequence of the fact that the function $\psi_x : \mathbf{M} \to f^T(x)\mathbf{M}^{-1} f(x)$ is convex on $\mathcal{S}^m_{++}$ (see [17], p. 62).
■

Naturally, we would use the full potential of Proposition 61 if we knew $\mathbf{M}_0$, simply setting $\mathcal{P} = \{\mathbf{M}_0\}$. However, we rarely can find the value of the D-optimal information matrix exactly. Nevertheless, as we show in the next section, we are able to construct a polyhedral set $\mathcal{P} = \operatorname{conv}\{\mathbf{Q}_1, ..., \mathbf{Q}_r\} \subseteq \mathcal{S}^m_{++}$ containing $\mathbf{M}_0$ *without* knowing $\mathbf{M}_0$. The set shall depend only on an information matrix $\mathbf{M} = \mathbf{M}(\xi)$, which is "close" to $\mathbf{M}_0$, i.e. on a suboptimal design ξ.

11.2 Construction of the double-simplex cage

In this section, we will describe a method of construction of a polyhedral set $\mathcal{P} \subseteq \mathcal{S}^m_{++}$ containing the D-optimal information matrix $\mathbf{M}_0$.

Choose any matrix $\mathbf{M} = \mathbf{M}(\xi) \in \mathcal{S}^m_{++}$. It is clear that $\mathbf{M}_0$ is an element of

$$\mathcal{C}_{\mathbf{M}} = \Big\{\mathbf{A} \in \mathcal{S}^m_+ : \det(\mathbf{A}) \geq \det(\mathbf{M})\Big\}.$$

Next, for $\xi \in \Xi$ we can write

$$\begin{aligned} \operatorname{tr} \mathbf{M}_0\mathbf{M}^{-1} &= \operatorname{tr}\Big(\textstyle\sum_{x;\xi^*(x)>0} \xi^*(x) f(x) f^T(x)\mathbf{M}^{-1}\Big) = \\ &= \textstyle\sum_{x;\xi^*(x)>0} \xi^*(x) f^T(x)\mathbf{M}^{-1} f(x) \leq \sup_{x\in\mathfrak{X}} f^T(x)\mathbf{M}^{-1} f(x), \end{aligned}$$

which means that $\mathbf{M}_0$ also belongs to

$$\mathcal{H}_{\mathbf{M}}(c) = \Big\{\mathbf{S} \in \mathcal{S}^m : \operatorname{tr} \mathbf{S}\mathbf{M}^{-1} \leq c + m\Big\},$$

where

$$c = \sup_{x\in\mathfrak{X}} f^T(x)\mathbf{M}_0^{-1} f(x) - m \geq 0.$$

Notice, that $\mathcal{H}_{\mathbf{M}}(c)$ has a simple geometric interpretation: it is the minimal half-space in $\mathcal{S}^m$ from all the half-spaces which contain $\mathcal{M}$ and which have the normal vector equal to $\nabla \ln \det(\mathbf{M}) = \mathbf{M}^{-1}$.

Consider the set

$$\mathcal{B}_{\mathbf{M}}(c) = \mathcal{C}_{\mathbf{M}} \cap \mathcal{H}_{\mathbf{M}}(c).$$

This set is closed, convex, and contains $\mathbf{M}_0$. Moreover, $\mathcal{B}_{\mathbf{M}}(c)$ is bounded, which is a simple consequence of a proposition proven in the sequel.

Let us introduce the function:

$$\varphi_{\mathbf{M}} : \mathcal{S}^m \to \mathcal{S}^m;\ \varphi_{\mathbf{M}}(\mathbf{S}) = \mathbf{M}^{-1/2}\mathbf{S}\mathbf{M}^{-1/2}.$$

One can see that the function $\varphi_{\mathbf{M}}$ is linear, regular (bijective), $\varphi_{\mathbf{M}}(\mathcal{S}^m_{++}) = \mathcal{S}^m_{++}$, and $\varphi_{\mathbf{M}}(\mathbf{M}) = \mathbf{I}_m$. This function allows us to normalize the problem, because $\varphi_{\mathbf{M}}(\mathcal{C}_{\mathbf{M}}) = \mathcal{C}_{\mathbf{I}_m}$, $\varphi_{\mathbf{M}}(\mathcal{H}_{\mathbf{M}}(c)) = \mathcal{H}_{\mathbf{I}_m}(c)$, resp. $\varphi_{\mathbf{M}}(\mathcal{B}_{\mathbf{M}}(c)) = \mathcal{B}_{\mathbf{I}_m}(c)$, which is easy to check. Therefore, it suffices to study the set

$$\mathcal{B}_{\mathbf{I}_m}(c) = \left\{\mathbf{A} \in \mathcal{S}^m_+ : \det(\mathbf{A}) \geq 1 \text{ and } \operatorname{tr}(\mathbf{A}) \leq m + c\right\}.$$

Lemma 62 *Let $m \geq 2$. Then for any $\mathbf{A} \in \mathcal{B}_{\mathbf{I}_m}(c)$, such that $\operatorname{tr}(\mathbf{A}) = m + c$:*

$$\left\|\mathbf{A} - \left(1 + \tfrac{c}{m}\right)\mathbf{I}_m\right\|_F \leq r_m(c), \text{ where } r_m(c) = \sqrt{\tfrac{m-1}{m}c^2 + (m^2 - m)c}.$$

Proof. Let $\mathbf{A} \in \mathcal{B}_{\mathbf{I}_m}(c)$, $\operatorname{tr}(\mathbf{A}) = m + c$, $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$, where $\mathbf{U}$ is the orthonormal matrix of eigenvectors of $\mathbf{A}$, and $\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, ..., \lambda_m)$, where $\lambda_1, ..., \lambda_m$ are corresponding eigenvalues of $\mathbf{A}$. The inequality $1 \leq \det(\mathbf{A}) = \prod_k \lambda_k$ and the relation between geometric and arithmetic means implies that for any $i \neq j$, $i, j \in \{1, ..., m\}$:

$$1 \leq ((\lambda_i\lambda_j) \prod_{k\neq i, k\neq j} \lambda_k)^{m-1} \leq \tfrac{1}{m-1}((\lambda_i\lambda_j) + \sum_{k\neq i, k\neq j} \lambda_k)$$

Summing up all the $\binom{m}{2}$ inequalities for $i < j$, and noticing that $\sum\limits_{i<j} \sum\limits_{k\neq i, k\neq j} \lambda_k = \binom{m-1}{2} \sum\limits_i \lambda_i$ we obtain:

$$\binom{m}{2}(m-1) - \binom{m-1}{2} \sum_i \lambda_i \leq \sum_{i<j} \lambda_i\lambda_j$$

From the previous inequality, the equality $\operatorname{tr}(\mathbf{A}^2) = \sum\limits_i \lambda_i^2 = \left(\sum\limits_i \lambda_i\right)^2 - 2\sum\limits_{i<j} \lambda_i\lambda_j$, and $\operatorname{tr}(\mathbf{A}) = \sum_i \lambda_i = m + c$, we get:

$$\left\|\mathbf{A} - \left(1 + \tfrac{c}{m}\right)\mathbf{I}_m\right\|_F^2 = (m+c)^2 - 2\sum_{i<j} \lambda_i\lambda_j - 2(1 + \tfrac{c}{m})(m+c) + m(1 + \tfrac{c}{m})^2 \leq$$
$$(m+c)^2 - 2\left(\binom{m}{2}(m-1) - \binom{m-1}{2}(m+c)\right) - 2(1 + \tfrac{c}{m})(m+c) + m(1 + \tfrac{c}{m})^2 =$$
$$\tfrac{m-1}{m}c^2 + (m^2 - m)c \ \blacksquare$$

Proposition 63 *Let $m \geq 2$. Then $\mathcal{B}_{\mathbf{I}_m}(c)$ is a subset of $\mathcal{R} = \operatorname{conv}(\mathcal{R}_* \cup \mathcal{R}^*)$, where*

$$\mathcal{R}^* = \left\{\mathbf{A} \in \mathcal{S}^m : \left\|\mathbf{A} - \left(1 + \tfrac{c}{m}\right)\mathbf{I}_m\right\|_F \leq r_m(c), \text{ and } \operatorname{tr}(\mathbf{A}) = m + c\right\}, \text{ and}$$
$$\mathcal{R}_* = \mathcal{R}^* - \tfrac{c}{m}\mathbf{I}_m.$$

Proof. It is simple to verify the proposition for $c = 0$. Let $c > 0$, $\mathbf{A} \in \mathcal{B}_{\mathbf{I}_m}(c)$, $\mathbf{R}^* = \mathbf{A} + \left(1 + \frac{c}{m}\right)\mathbf{I}_m - \left(\frac{1}{m}\operatorname{tr}(\mathbf{A})\right)\mathbf{I}_m$, $\mathbf{R}_* = \mathbf{R}^* - \frac{c}{m}\mathbf{I}_m$, and $\beta = \frac{1}{c}(m + c - \operatorname{tr}(\mathbf{A}))$. Notice, that $\operatorname{tr}(\mathbf{R}^*) = m+c$, and $\mathbf{R}^* \geq \mathbf{A}$ in Loewner ordering, therefore $\det(\mathbf{R}^*) \geq \det(\mathbf{A}) \geq 1$. Consequently, the previous lemma entails $\mathbf{R}^* \in \mathcal{R}^*$, and hence also $\mathbf{R}_* \in \mathcal{R}_*$. Obviously $\beta \in [0, 1]$, because $m \leq \operatorname{tr}(\mathbf{A}) \leq m + c$. Moreover, $\beta\mathbf{R}_* + (\mathbf{1} - \beta)\mathbf{R}^* = \mathbf{R}^* - \beta\frac{c}{m}\mathbf{I}_m = \mathbf{A}$, as is easy to check.

■

The set $\mathcal{R}$ from the previous proposition forms a multi-dimensional cylinder, because the $k = \frac{1}{2}m(m+1) - 1$ dimensional circles $\mathcal{R}_*$ and $\mathcal{R}^*$ are parallel. Hence, we are able to encase $\mathcal{R}$ into a convex polyhedral set generated by $2k+2 = m(m+1)$ symmetric matrices $\mathbf{R}_1, ..., \mathbf{R}_{2k+2}$, where $\mathbf{R}_1, ..., \mathbf{R}_{k+1}$ are vertices of a simplex circumscribing $\mathcal{R}_*$, and $\mathbf{R}_{k+2} = \mathbf{R}_1 + \frac{c}{m}\mathbf{I}_m, ..., \mathbf{R}_{2k+2} = \mathbf{R}_{k+1} + \frac{c}{m}\mathbf{I}_m$ are vertices of a simplex circumscribing $\mathcal{R}^*$. (Naturally, this construction is a compromise between the volume and the number of vertices; we can construct a polyhedral supperset of $\mathcal{R}$ with somewhat smaller volume but with more vertices.)

It is obvious that we can construct the matrices $\mathbf{R}_1, ..., \mathbf{R}_{2k+2}$ as follows:

$$\mathbf{R}_i = k.r_m(c).\mathbf{A}_i + \mathbf{I}_m,\ \mathbf{R}_{i+k+1} = \mathbf{R}_i + \tfrac{c}{m}\mathbf{I}_m \text{ for } i = 1, ..., k+1,$$

where $\mathbf{A}_1, ..., \mathbf{A}_{k+1}$ correspond to the vertices of a regular simplex circumscribed by the unit sphere in the k dimensional linear space $\mathbf{I}_m^{\perp} \cap \mathcal{S}^m$, that is $\mathbf{A}_1, ..., \mathbf{A}_{k+1}$ are symmetric matrices which satisfy: $\langle \mathbf{A}_i, \mathbf{A}_j \rangle = \mathrm{tr}(\mathbf{A}_i\mathbf{A}_j) = -1/k$ for all $i \neq j$, $\langle \mathbf{A}_i, \mathbf{I}_m \rangle = \mathrm{tr}(\mathbf{A}_i) = 0$, and $\|\mathbf{A}_i\|_F = \sqrt{\mathrm{tr}(\mathbf{A}_i^2)} = 1$ for all $i = 1, ..., k+1$.

Transforming the vertices $\mathbf{R}_1, ..., \mathbf{R}_{2k+2}$ by $\varphi_{\mathbf{M}}^{-1}$, and summarizing all the pertinent results above, we obtain the following theorem:

Theorem 64 *([7]) Let* $\mathbf{M} \in \mathcal{M} \cap \mathcal{S}_{++}^m$, $k = \frac{1}{2}m(m+1) - 1$,

$$c = \sup_{x \in \mathfrak{X}} f^T(x)\mathbf{M}^{-1}f(x) - m, \text{ and } r = \sqrt{\frac{m-1}{m}c^2 + (m^2 - m)c}.$$

Next, let $\mathbf{A}_1, ..., \mathbf{A}_{k+1}$ *be a set of symmetric matrices of the type* $m \times m$ *which satisfy:* $\langle \mathbf{A}_i, \mathbf{I}_m \rangle = 0$, $\|\mathbf{A}_i\|_F = 1$, $\langle \mathbf{A}_i, \mathbf{A}_j \rangle = -1/k$ *for all* $i \neq j$, $i, j = 1, ..., k+1$. *Define*

$$\mathcal{P} = \mathrm{conv}\left\{\mathbf{Q}_1, ..., \mathbf{Q}_{m(m+1)}\right\},$$

where

$$\mathbf{Q}_i = k.r.\mathbf{M}^{1/2}\mathbf{A}_i\mathbf{M}^{1/2} + \mathbf{M},\ \mathbf{Q}_{i+k+1} = \mathbf{Q}_i + \frac{c}{m}\mathbf{M}, \text{ for } i = 1, ..., k+1.$$

Then the D-optimal information matrix belongs to $\mathcal{P}$. *Moreover, if* $k.r < 1$ *then* $\mathcal{P} \subseteq \mathcal{S}_{++}^m$.

Proof. The fact that $\mathbf{M}_0 \in \mathcal{P}$ follows from Proposition 63 and the considerations above. We shall prove that $k.r < 1$ implies $\mathcal{P} \subseteq \mathcal{S}_{++}^m$. Clearly, it is enough to guarantee that $\mathbf{A}_i + \mathbf{I}_m$ are positive semidefinite for all $i = 1, ..., k+1$. To prove this, we denote the eigenvalues of $\mathbf{A}_i$ by $\gamma_1, ..., \gamma_m$ then $1 = \mathrm{tr}(\mathbf{A}_i^2) = \sum_j \gamma_j^2$, which means $\gamma_j \geq -1$ for all $j = 1, ..., m$. But the eigenvalues of $\mathbf{A}_i + \mathbf{I}_m$ are $\gamma_1 + 1, ..., \gamma_m + 1$. Consequently, the symmetric matrix $\mathbf{A}_i + \mathbf{I}_m$ has all the eigenvalues nonnegative, hence it is positive semidefinite.

■

An important fact to notice is that $\mathbf{M} \to \mathbf{M}_0$ implies $c \to 0$ which in turn guarantees that $r_m(c) \to 0$. Therefore, the condition $k.r < 1$ shall be satisfied if $\mathbf{M}$ is close enough to $\mathbf{M}_0$, and we shall have $\mathcal{P} \subseteq \mathcal{S}^m_{++}$. Also, the diameter of $\mathcal{P}$ converges to 0 as $\mathbf{M} \to \mathbf{M}_0$, although the convergence is relatively slow: $\operatorname{diam}\mathcal{P} \lesssim \text{constant}\,.\sqrt{c}$ for the values of c approaching 0.

The matrices $\mathbf{A}_1, ..., \mathbf{A}_{k+1}$ in Theorem 64 depend only on the number m of parameters, so we need to compute them only once. Moreover, there exists a very fast (finite) iterative method how to find a set of such matrices, as we will outline.

Consider the following system of $2k$ equalities (the symbols $a_1, ..., a_k, d_1, ..., d_k$ represent unknowns):

$$\begin{array}{l} a_1 = 1,\ a_1 d_1 = -\frac{1}{k}, \\ d_1^2 + ... + d_{i-1}^2 + a_i^2 = 1 \text{ for } i = 2, ..., k, \\ d_1^2 + ... + d_{i-1}^2 + a_i d_i = -\frac{1}{k} \text{ for } i = 2, ..., k. \end{array}$$

It is not difficult to show that this system has a unique vector of solutions $(\alpha_1, ..., \alpha_k, \delta_1, ..., \delta_k) \in \Re^{2k}$, such that $\alpha_i \geq 0$ for all $i = 1, ..., k$ and that the solutions satisfy:

$$\delta_1^2 + ... + \delta_{k-1}^2 - \alpha_k^2 = -\frac{1}{k}$$

Note, that it is simple to derive the solutions if we keep the order of calculations given by a scheme

$$\alpha_1 \to \delta_1 \to \alpha_2 \to \delta_2 \to ... \to \alpha_k \to \delta_k$$

Thus, for example if $p = 2$ $(k = 2)$ we get the solution $\left(1, \sqrt{3}/2, -1/2, -\sqrt{3}/2\right)$, and for $p = 3$ $(k = 5)$ we obtain

$$1/10 \times \left(10, \sqrt{96}, \sqrt{90}, \sqrt{80}, \sqrt{60}, -2, -\sqrt{6}, -\sqrt{10}, -\sqrt{20}, -\sqrt{60}\right)$$

Let $\mathbf{B}_1, ..., \mathbf{B}_k$ be any orthonormal basis of $\mathbf{I}_m^{\perp} \cap \mathcal{S}^m$. The method of construction of scalars α_i and δ_i guarantees that we can construct the vertices of the simplex as:

$$\begin{array}{l} \mathbf{A}_1 = \alpha_1 \mathbf{B}_1, \\ \mathbf{A}_i = \delta_1 \mathbf{B}_1 + ... + \delta_{i-1}\mathbf{B}_{i-1} + \alpha_i \mathbf{B}_i \text{ for } i = 2, ..., k, \\ \mathbf{A}_{k+1} = \delta_1 \mathbf{B}_1 + ... + \delta_{k-1}\mathbf{B}_{k-1} - \alpha_k \mathbf{B}_k. \end{array}$$

For example, if $m = 2$ $(k = 2)$ we can choose

$$\mathbf{B}_1 = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \mathbf{B}_2 = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and the method described above gives

$$\mathbf{A}_1 = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \mathbf{A}_2 = \tfrac{1}{2\sqrt{2}} \begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \mathbf{A}_3 = \tfrac{1}{2\sqrt{2}} \begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}.$$

The computation of the matrices $\mathbf{Q}_i$ from Theorem 64 is thus algorithmically simple and rapid. Consequently, according to Proposition 61, the matrices $\mathbf{Q}_i$ can be used to delete those points from the experimental domain, which can not support any D-optimal design.

11.3 Example: Cubic regression without an intercept term

As an illustrative example we have chosen the problem of a D-optimal design for the linear regression model given by the formula

$$y = \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \varepsilon,$$

where the values x are from the experimental domain $\mathfrak{X} = \{0, 0.1, 0.2, ..., 4.9, 5.0\}$.

For the computation of a D-optimal design, we will use an algorithm, which is specially suited for a discrete design space ([29]). We shall begin with the uniform initial design $\xi_{(0)}$; $\xi_{(0)}(x) = 1/51$ for all $x \in \mathfrak{X}$. Then we shall perform the iterations setting at the step number $n = 0, 1, 2, ...$:

$$\xi_{(n+1)}(x) = \frac{1}{m}\xi_{(n)}(x). \left[f^T(x)\mathbf{M}\left(\xi_{(n)}\right)^{-1} f(x) \right] \text{ for all } x \in \mathfrak{X}$$

Evidently, in any iteration of the algorithm we have $\xi_{(n)}(x) > 0$ for all $x \in \mathfrak{X} \setminus \{0\}$. It means that the algorithm (resp. a computer program) must take all the points (except of 0) into account, even when the majority of weights of $\xi_{(n)}$ are negligibly small. Naturally, the computations with very small positive values take approximately as much time as those with large real numbers. The method described in the previous sections allows us to remove many such points, and consequently speed up the computations.

More precisely, we incorporated a modification to the algorithm, such that at every 100-th step, we remove all the points $x \in \mathfrak{X}$ for which

$$\max_{i=1,...,12} f^T(x)\mathbf{Q}_i^{-1} f(x) < 3$$

where the matrices $\mathbf{Q}_i$ are defined in Theorem 64. After each removal of points from the support of $\xi_{(n)}$, we standardized the remaining measure to 1.

At Figure 8 we see which points were removed (grey dots) and kept (black dots) at each iteration. (The vertical axis corresponds to $\mathfrak{X}$ and the horizontal axis represents the number of iterations.) Notice that we finally arrived at a 3-point support, which is the smallest size possible. After the last deletion, the convergence of weights was very rapid, shortly arriving at the optimal design - the uniform probability on $\{1.4, 3.6, 5.0\}$ - within the limits of the numerical precision of the software.

While the overall speed of convergence was observed to be higher using the deletion method, the number of iterations needed to obtain a given precision was almost the same as for the unmodified algorithm (except of the very final stage with the support identified by the deletion method exactly). The deletions usually remove points with very small weights, hence they do not change the quality of the design significantly.

Chapter 12
APPENDIX

12.1 Graphs

Figure 1 A lower bound on the $\mathbb{O}$-minimal efficiency of D-optimal designs depending on the eigenvalues of the information matrix (see Theorem 34).

Figure 2 A lower bound on the $\mathbb{O}$-minimal efficiency of A-optimal designs depending on the eigenvalues of the information matrix (see Theorem 34).

Figure 3 The model from Chapter 8, degree 2. The bounds for the $\mathbb{O}$-minimal efficiency of the D-optimal design (solid line). The $\mathbb{O}$-minimal efficiency of the E-optimal design (dashed line). (See Theorem 59)

Figure 4 The model from Chapter 8, degree 8. The bounds for the $\mathbb{O}$-minimal efficiency of the D-optimal design (solid line). The $\mathbb{O}$-minimal efficiency of the E-optimal design (dashed line). (See Theorem 59.)

Figure 5 The E_1, E_2, E_3 and the $\mathbb{O}$-minimal efficiency of $\Phi_{p(r)}$-optimal designs for the quadratic polynomial regression model. (See Chapter 10.)

Figure 6 The E_1, E_2, E_3, E_4 and the $\mathbb{O}$-minimal efficiency of $\Phi_{p(r)}$-optimal designs for the cubic polynomial regression model. (See Chapter 10.)

Figure 7 The E_1, E_2, E_3, E_4, E_5 and the $\mathbb{O}$-minimal efficiency of the $\Phi_{p(r)}$-optimal designs for the biquadratic polynomial regression model. (See Chapter 10.)

Figure 8 Deletion of points which do not support a D-optimal design for the cubic polynomial regression without an intercept term. (See Section 11.3.)

12.2 Notation

$\mathfrak{R}$	set of all real numbers
$\mathfrak{R}^m_+$	set of m-dimensional vectors with nonnegative real components
$\mathfrak{R}^m_{++}$	set of m-dimensional vectors with positive real components
$\mathfrak{R}^m_{\leq}$	set of m-dimensional vectors with components in a nondecreasing order
$\mathfrak{N}$	set of natural numbers
$\mathfrak{E}_{f,\mathfrak{X}}$	Elfving set corresponding to the model $(f,\mathfrak{X})$
$\mathrm{span}(\mathfrak{H})$	set of all linear combinations of vectors in $\mathfrak{H} \subseteq \mathfrak{R}^m$
$\mathrm{conv}(\mathfrak{H})$	set of all convex combinations of vectors in $\mathfrak{H}$ (the convex hull of $\mathfrak{H}$)
$\mathrm{diam}(\mathfrak{H})$	supremal Euclidean distance of vectors in $\mathfrak{H}$ (the diameter of $\mathfrak{H}$)
$\mathcal{S}^m$	set of symmetric matrices of type $m \times m$
$\mathcal{S}^m_+$	set of positively semidefinite symmetric matrices of type $m \times m$
$\mathcal{S}^m_{++}$	set of positively definite symmetric matrices of type $m \times m$
$\mathcal{U}_{m,k}$	set of matrices of type $m \times k$ with orthonormal columns
$\mathcal{P}_{m,k}$	set of all orthogonal projectors of type $m \times m$ and rank k
$\mathcal{M}_{f,\mathfrak{X}}$	set of all information matrices for the model $(f,\mathfrak{X})$
$\lambda(\mathbf{A})$	vector of eigenvalues of the matrix $\mathbf{A} \in \mathcal{S}^m$ in a nondecreasing order
$\lambda_{\downarrow}(\mathbf{A})$	vector of eigenvalues of the matrix $\mathbf{A} \in \mathcal{S}^m$ in a nonincreasing order
$\lVert\mathbf{A}\rVert_F$	Frobenius (l_2) norm of the matrix $\mathbf{A} \in \mathcal{S}^m$
$\mathbf{I}_m$	identity matrix of type $m \times m$
$\mathbf{M}_{f,\mathfrak{X}}(\xi)$	information matrix of the design ξ for the model $(f,\mathfrak{X})$
1_m	vector $(1,...,1)^T \in \mathfrak{R}^m$
0_m	vector $(0,...,0)^T \in \mathfrak{R}^m$
$\mathrm{diag}(a)$	diagonal matrix with elements of the vector a on the diagonal
$\mathbb{O}$	set of all orthogonally invariant criteria
Φ_{E_k}	criterion of E_k-optimality
$\widetilde{\Phi}_{E_k}$	sum of the k smallest eigenvalues of a symmetric matrix
Φ_p	Kiefer's criterion of Φ_p-optimality, $p \in [-\infty, 1]$
$\nabla\Phi(\mathbf{A})$	gradient of the function Φ in $\mathbf{A}$
$\partial\Phi(\mathbf{A})$	subdifferential of the concave function Φ in $\mathbf{A}$
$v_{f,\mathfrak{X}}(k)$	E_k-optimal value of the model $(f,\mathfrak{X})$
$\mathrm{eff}_{f,\mathfrak{X}}(\xi : \zeta \mid \Phi)$	efficiency of ξ relative to ζ for $(f,\mathfrak{X})$ with respect to Φ
$\mathrm{eff}_{f,\mathfrak{X}}(\xi \mid \Phi)$	absolute efficiency of the design ξ for $(f,\mathfrak{X})$ with respect to Φ
$\mathrm{mineff}_{f,\mathfrak{X}}(\xi \mid \mathbb{O})$	$\mathbb{O}$-minimal efficiency of the design ξ for the model $(f,\mathfrak{X})$

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